AHPCRC

Army High Performance Computing Research Center

ARL

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AHPCRC Consortium Members

U.S. Army Research Laboratory
Stanford University
High Performance Technologies, Inc.
Morgan State University
NASA Ames Research Center
New Mexico State University at Las Cruces
The University of Texas at El Paso

www.ahpcrc.org

AHPCRC, The Army High Performance Computing Research Center, is a cooperative agreement between the U.S. Army Research Laboratory (ARL) and a consortium of university and industry partners. AHPCRC exploits high performance computing (HPC) to addresses the Army's most difficult scientific and engineering challenges. Consortium researchers work in close partnership with researchers at Army Research Development and Engineering Command (RDECOM), Engineering Research and Development Center (ERDC), and Medical Research and Materiel Command (MRMC) to exchange information, conduct collaborative research, validate their models against laboratory studies, and maintain alignment between their research and the problems of greatest interest to the U.S. Army. Computational capabilities and associated HPC software developed under AHPCRC are transitioned to Army researchers. These capabilities are continually developed to provide problem-solving capabilities required to pursue RDECOM's vision to be the world leader in rapid and innovative research, development, and engineering for the warfighter.

High performance computing enables the development of high fidelity computer models that provide significant advantages in designing and characterizing complex systems involving many interacting factors. Validated high fidelity computer simulations reduce the time and expense of designing, optimizing, and characterizing complex systems. This, in turn, enables decision-makers to prioritize design trade-offs and to make informed acquisition decisions.

Realistic computer simulations and models enable a sophisticated and intentional approach to the design, characterization, and optimization of complex systems. Many combinations of parameters and variables can be tested, leading to solutions that might not have been foreseen by the researcher. As applied science and engineering problems become more complex, computing capabilities must keep up with the demand. Existing codes must be adapted to run on parallel computing systems, operate on multiple platforms, and be easily transferred to newer systems as they arise. Software must be comprehensible and applicable to the intended users.

AHPCRC seeks to develop the potential of HPC capabilities and applications as a means of addressing the real-world needs of today's warfighter: strong, lightweight protective gear; agile unmanned aerial surveillance vehicles; early-warning systems for biowarfare agents; better medical treatments; lightweight vehicle and ammunition components; efficient wireless network designs; and rapid, secure data aggregation and dissemination.

In addition, AHPCRC fosters the education of the next generation of scientists and engineers—including those from racially and economically disadvantaged backgrounds—in the fundamental theories and best practices of simulation-based engineering sciences and high performance computing.

Dr. Raju R. Namburu

AHPCRC Cooperative Agreement Manager

Army Research Laboratory AHPCRC

Contents

"To further individual soldier protection systems, Army S&T is pursuing improvements in body armor component fabrics and materials through two technical design paths. The first path will provide increased levels of protection at equal weight and/or in better, flexible configurations. The second path will provide the same level of protection at significantly reduced weights. For both designs, performance enhancements will be achieved through advances in high performance ballistic fiber and textile technologies, transparent polymers, composites, and materials systems integration. For example, Army S&T efforts are currently focused on improving the high performance ballistic fiber technology needed to obtain a 50% increase in textile material strength to reduce soft body armor weight by 40-50%." — *Dr. Thomas H. Killion*

Force Protection

Lightening the Soldier's Load

Power and Energy
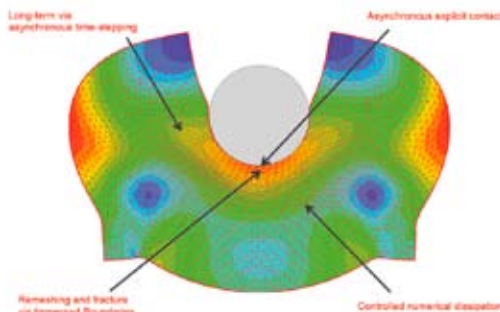
"S&T investments contributing to soldier weight reduction [include increasing capabilities in] powered equipment and battery weight reduction (efficient batteries, night vision, communications and sight augmentation systems)…"

"As the emphasis on deployed forces is placed more on light infantry type operations, continued investment and maturation of materials and processes to lighten the load on individual Soldiers is paramount to a target goal of achieving true fighting load weights for all Soldiers regardless of specialized weapons or communications."

Ballistic impact research aids in the design of strong, lightweight armoring materials, including fabrics used to line personal protective gear and vehicle wheel wells. Insights into the effects of ballistic impact on deformable materials such as polymers can be applied to similar effects in human tissues, thus aiding the development of wound treatments and reconstructive surgeries.

High performance computer simulation allows designers to try out numerous mechanical and material configurations, without the time and expense of building multiple physical models. Computer models aid in understanding the rapid sequence of events associated with ballistic impact. Simulations enable systematic evaluations that are not practical with live subjects.

Clockwise from top left: Ballistic fabric impact simulation (C. Farhat, Stanford; T. Zohdi, UC Berkeley). Impact simulation for ballistic gel (A. Lew, Stanford). Electron density map for the all-electron battery (F. Prinz, Stanford). Dislocation distribution and orientation in metal thin films (W. Cai, Stanford). Electron micrograph of dislocation patterns in metal. (W. Cai, Stanford).
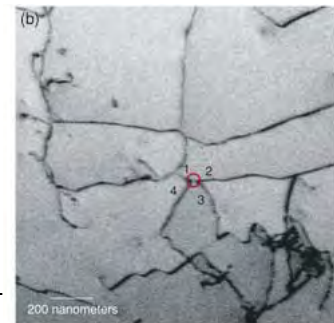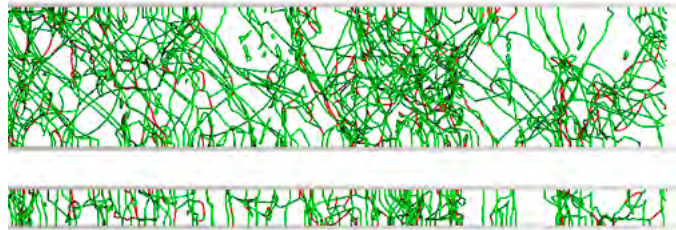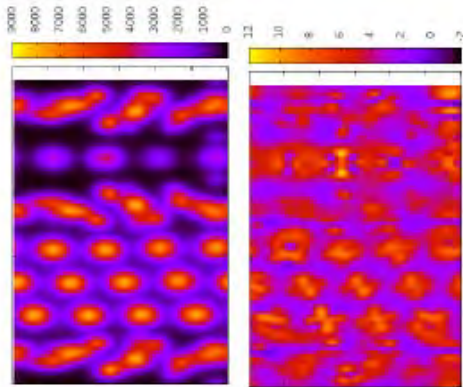
Military field gear and remote operations increasingly rely on portable power sources, but storing and transporting batteries can pose a significant burden on military operations. Portable power is crucial for a range of military operations. Energy-dense batteries would increase soldier mobility and lessen transportation costs. The all-electron battery shows promise with respect to high energy density, power density, and battery lifetime.

High performance computer modeling and simulation can augment and guide device design and evaluation, not only by simulating various configurations and materials, but by assisting in understanding the basic physical principles involved in charge transfer and storage on a quantum mechanical level.

Performance for miniature electronic devices is often limited by material defects. Several technologies of interest to the Army, including handheld spectrometers, inter-subband cascade lasers, next-generation solar cells, and high resolution imaging satellites, are currently limited by low pixel operability and energy localization due to dislocations within the central detector element (usually a charge-coupled device).

High performance computing can create detailed, high-fidelity models of dislocation dynamics in metal and semiconductor films. These models can be made specific for thin films, pillars, and other structures in the nano-scale regime, which is poorly understood at present. HPC resources are vital to extending these models beyond static structures to include the rate-dependent response of miniature mechanical components to external loading.
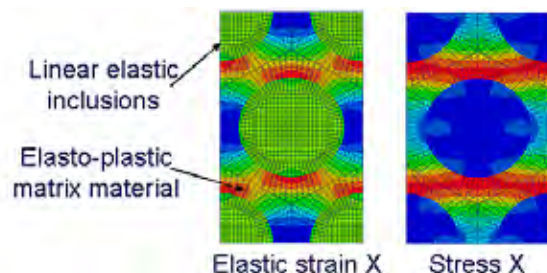
Project 1–1: Multifield Simulation of Accelerated Environmental Degradation of Fabric, Composite, and Metallic Shields and Structures

Principal Investigators: Tarek Zohdi (University of CA – Berkeley) and Charbel Farhat (Stanford University)

Simulations of deformation behavior for composite ballistic shielding material. (G. Mseis and T. Zohdi, UC Berkeley)

Adequately protecting soldiers without weighing them down unnecessarily is one of the Army's greatest technological and operational challenges. Lightweight protective fabrics must reduce human casualties and damage to equipment and vehicles, while standing up to the effects of weathering and prolonged storage.

Full-scale experimental tests of these materials, especially in large-scale applications such as vehicle and structure protection, can be extremely time consuming and expensive. A fast, reliable computational approach enabled by high performance computing (HPC) is an ideal alternative. Computer models assist designers in trying out new configurations and understanding fabric properties.

AHPCRC researchers are developing advanced computer models of multifunctional ballistic fabrics, alone and attached to rigid supports. They are creating simulations of ballistic impact on these fabrics, which produces multiple physical effects at high speeds. HPC simulations, using parallel code to model nonlinear solid dynamics, allow researchers to examine material failures frame-by-frame, and to test various components singly or in groups. Simulations may suggest effective material configurations that are not intuitively obvious from experimental data alone.

AHPCRC researchers are adapting existing simulation codes for use in parallel processing applications and finite element analysis. They are also building new capabilities, such as modeling damage from various types of projectiles, accounting for imperfections introduced during the weaving of fabrics, evaluating methods for attaching the protective fabric to an underlying structure, and simulating the propagation and growth of flaws in fabrics.

Current work focuses on modeling fiber-based composite materials and on modeling the effects of moisture absorption, heat, and mechanical damage on ballistic fabrics in laminated and metal-substrate systems. Results of the modeling study are being compared with laboratory tests performed at the University of California, Berkeley.

Simulated ballistic impact of projectile on fabric. (D. Powell and C. Farhat, Stanford)

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Lightweight Protection and Energy

Project 1–2: Simulation of Ballistic Gel Penetration

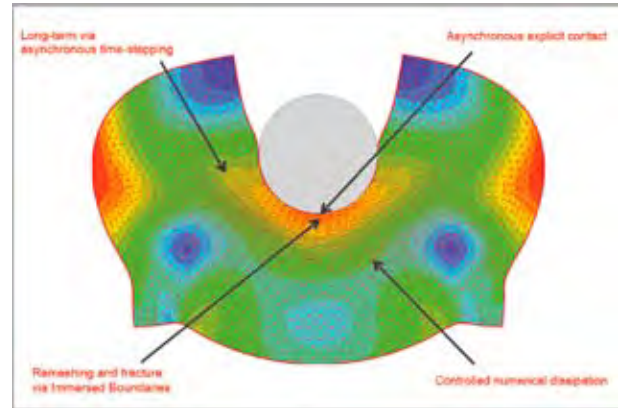Principal Investigator: Adrian Lew (Stanford University)

Ballistic impact on deformable materials like polymers and human soft tissues produces multiple physical effects at high speeds. Within a few milliseconds, these materials deform, crack, melt, and rupture at the site of the impact, and the effects are propagated to the surrounding areas and attached structures. Very little is known about the specific mechanisms by which soft materials fail after ballistic impact.

AHPCRC researchers are developing HPC computational tools to simulate how these materials respond to stress, impact, heat, and shock. This enables them to examine in detail the evolution of the cavity behind a projectile. They are working to extend their simulations to cover a period of 10–50 milliseconds after impact (a significant period of time in the world of computer simulations) and calculate the amount of energy involved in damaging the material. This will provide valuable insights for use in treating traumatic injuries and designing protective gear.

Ongoing work will address the effects of projectile shape and composition on the cavity it produces. As the project advances, factors such as projectile tumbling, erosion, and fragmentation inside the cavity can be factored in.
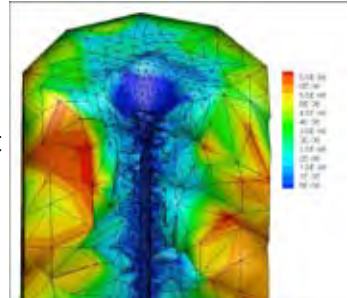

Top and bottom right: Simulated mechanical response of a ballistic gel tissue simulant to projectile impact. (A. Lew, Stanford)

The researchers have developed and released a verified parallel code, dubbed COMODIN++, for performing nonlinear solid dynamics simulations. This code is capable of fully asynchronous time stepping, allowing calculations in rapidly deforming regions of the solid to be performed in fine detail while using a coarser resolution in more stable areas.

Current research focuses on increasing the number of processors for the modeling and simulation runs, investigating the effect of techniques for simplifying the calculations (sending the projectile through a pre-existing hole, for example) on the accuracy of the results, and making the models more realistic by adding features such as material failure and energy dissipation effects. Results of the modeling studies are compared with laboratory tests on Permagel (a soft tissue simulant) performed at the University of California, Berkeley.

A projectile leaves a characteristic path in a ballistic gel, which simulates human tissue. (T. Zohdi, UC Berkeley)

Project 1–8: High-performance computation of projectile impact with electromagnetic fabric

Principal Investigators: Tarek I. Zohdi (University of California, Berkeley),
Charbel Farhat (Stanford University)

Electromagnetically-sensitive fabrics represent a potentially significant enhancement over traditional ballistic shielding fabrics. Contact with a projectile induces electromagnetic forces on the fabric that can cause the projectile to rotate, making it less likely to penetrate the fabric. A new generation of electromagnetically-enhanced ballistic fabric shielding for structures—and potentially body armor—could provide enhanced protection with little if any additional weight. High-performance algorithms will be developed, capable of treating the type of unique physics involving multiphysical contact, transient current flow through a fabric network, electromagnetic fabric deformation and rupture, and electromagnetically-induced thermodynamic heating.

(New project, 2010)
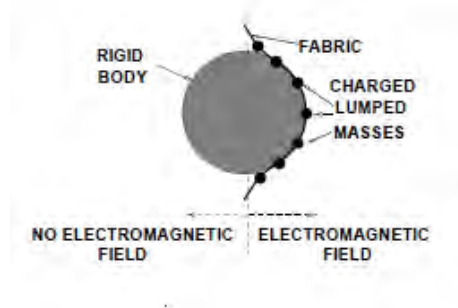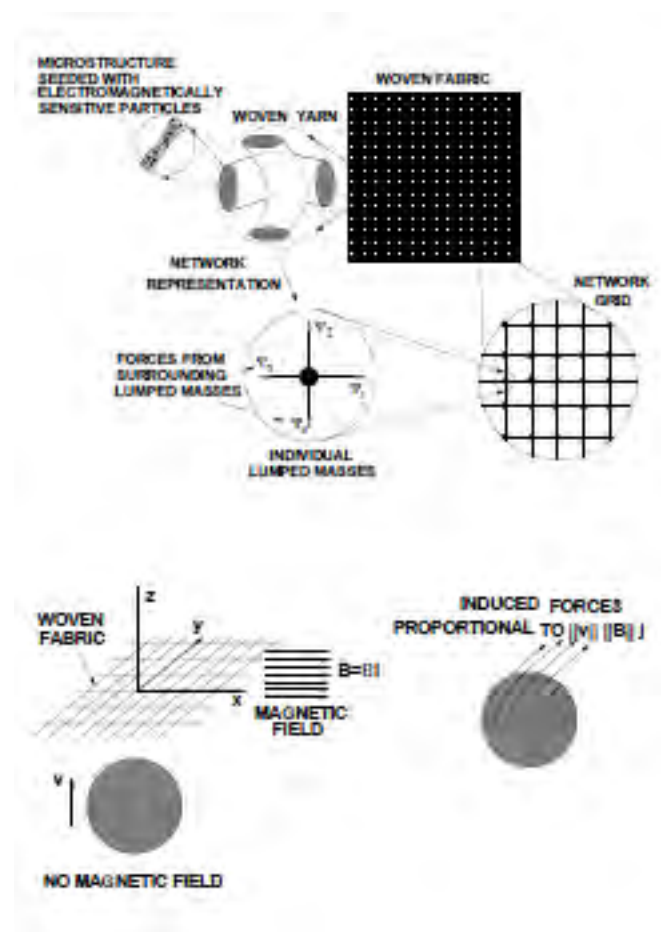
Clockwise from top right: 1) Woven ballistic fabric represented as a network. Projectile pushes an EM-sensitive fabric into a magnetic field. 2) Projectile impact on Kevlar fabric. 3) Schematic of the EM fabric concept. (Graphics: T. Zohdi, C. Farhat. Photograph: US Army RDECOM.)

Project 1–6: The All-Electron Battery: Quantum Mechanics of Energy Storage in Electron Cavities
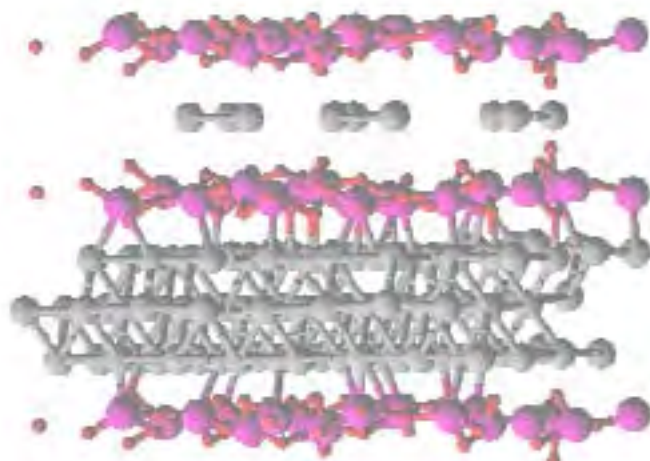
Principal Investigator: Fritz Prinz (Stanford University)

Portable power is crucial for a range of military operations. A soldier executing a 72 hour mission in Afghanistan must carry 26 pounds of batteries. A future battery with higher energy density could allow a soldier to carry more ammunition, body armor, other equipment, or be more mobile and suffer less fatigue.

The Rapid Prototyping Laboratory (RPL) at Stanford University is developing a new all-electron battery (AEB) with the potential to deliver significantly higher energy density than state-of-the-art lithium ion batteries. Recent experiments in the RPL have shown that this new battery may deliver both high power density and high energy density, and exhibit a longer lifetime than conventional batteries. The AEB stores energy in charge separation, using only electrons, which are lighter, and therefore faster, than the ion charge carriers typical of conventional batteries.

The RPL is currently fabricating and testing a proof-of-concept device. Ongoing research focuses on materials selection for each component of the device and testing the scalability of the device by adding more layers. To develop practical devices, charge transfer and storage in the AEB must be understood, and this is where HPC modeling and simulation come into play. A quantum mechanical approach, although computationally demanding, is necessary to formulate tests of various hypotheses and to make accurate predictions of AEB behavior.

Crystal structure of layered system ZrO_2 | Pt QW | ZrO_2 | $3Pt_3$ QDs | ZrO_2
(Graphics this page: F. Prinz, Stanford)

Charge density distribution before (left) and after (right) the system is charged with 4 extra electrons.
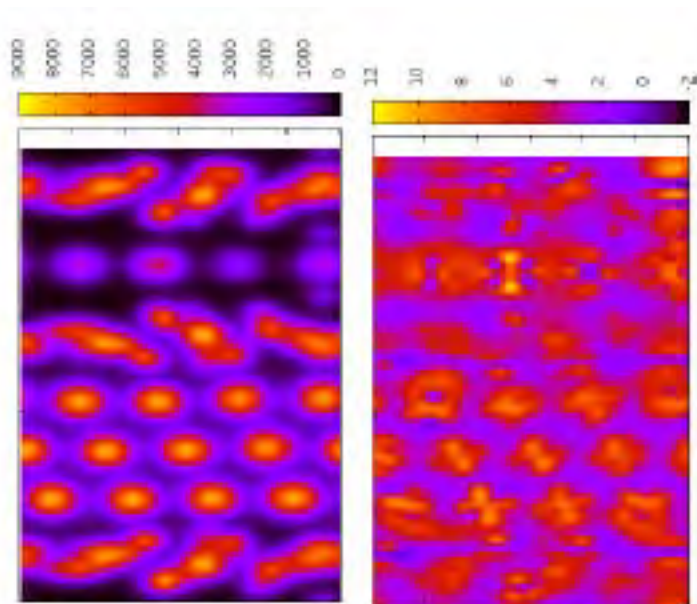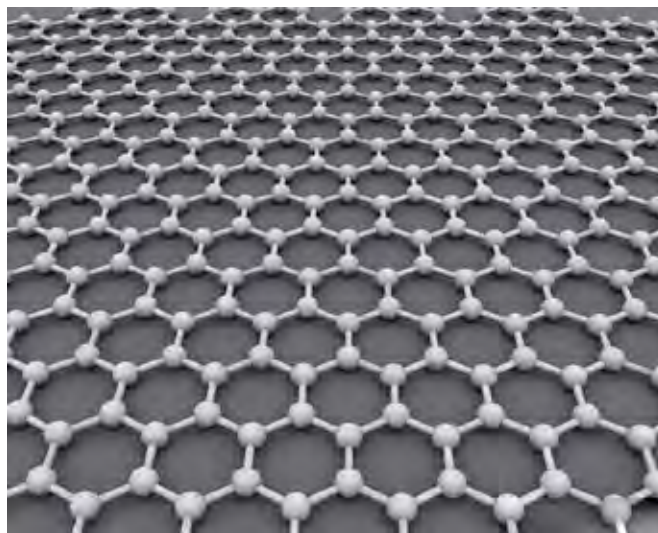
Project 2–7: Graphene Chemistry for Electronics Applications

Principal Investigator: Evan Reed (Stanford University)

The discovery of a practical manufacturing process for graphene (a form of carbon having a single graphite-structured atomic layer) shows great potential for the fabrication of 2D electronic devices. Current graphene devices are limited by chemical impurities and structural disorder effects. Mitigation of such effects would be of significant value in fabricating practical devices. Intentional addition of surface species could open useful avenues for reconfiguring the electrical, mechanical, optical and other properties of graphene devices. Using quantum approaches and molecular dynamics simulations, this project will determine the thermodynamically favorable arrangements of hydrogen around a graphene edge and graphene imperfections.

(New project, 2010)

Graphene structure. (Alexander AIUS, Wikimedia Commons.)

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**Lightweight Protection
and Energy**

# Project 2–5: Nanoscale Dislocation Dynamics in Crystals

Principal Investigator: Wei Cai (Stanford University)

Electronic devices made using microscopically-sized parts are often limited by material behaviors that are unique to that size scale. Handheld spectrometers, inter-subband cascade lasers, next-generation solar cells, and high-resolution imaging satellites are among the devices that are currently constrained by low pixel operability and energy localization arising from dislocations (crystal defects) within a central detector element.

Material behavior at small scales is an important predictor of the durability and useful lifetime of micro-electronic and micro-electromechanical devices (MEMS). Many of the mechanical properties of sub-micron-sized metal or semiconductor particles are size-dependent. These properties, including yield strength and resistance to fatigue, are not well predicted by macroscopic characterization.

Modeling and simulation tools guide materials scientists toward the best methods of producing durable, reliable nanoscale device components. Simulating such systems requires detailed models of materials with a high ratio of surface area to bulk material, the capability to simulate effects on a variety of size scales, and the inclusion of methods for simulating strain characteristics produced under varying stress rates.

ParaDiS (http://paradis.stanford.edu), a dislocation dynamics HPC code supported in part by AHPCRC, is being developed to simulate the plastic deformation of metal thin films and cylinders under high rates of strain. Efficient
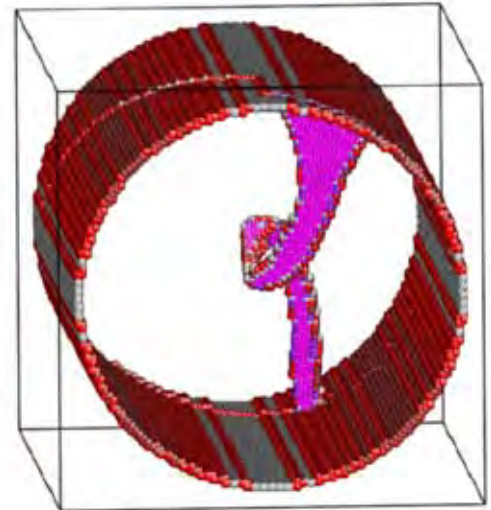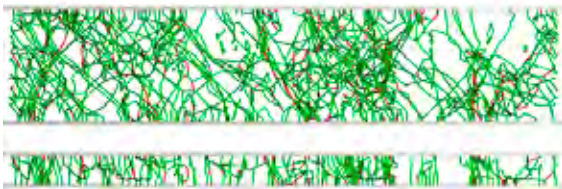
Top: Schematic of a dislocation with a jog. *Bottom left:* Dislocation distribution and orientation for thick and thin metal films. *Bottom right:* Micrographs of metal nanopillars. (Graphics this page: W. Cai, Stanford)

algorithms have been designed to simulate strain hardening effects and stresses from free surfaces in films.

The first direct comparison between the dislocation dynamics models and existing molecular dynamics models has been completed for dislocations in a free-standing thin film. When image stress (surface-related stress) is correctly accounted for, both types of models are in excellent agreement. The ParaDiS code was developed to model metals, but recent and upcoming work is focused on expanding it for use with semiconductor films as well.
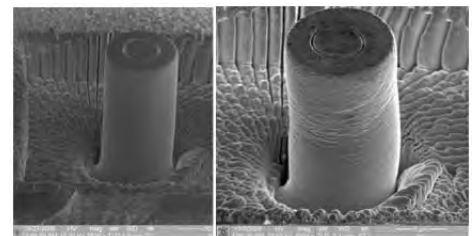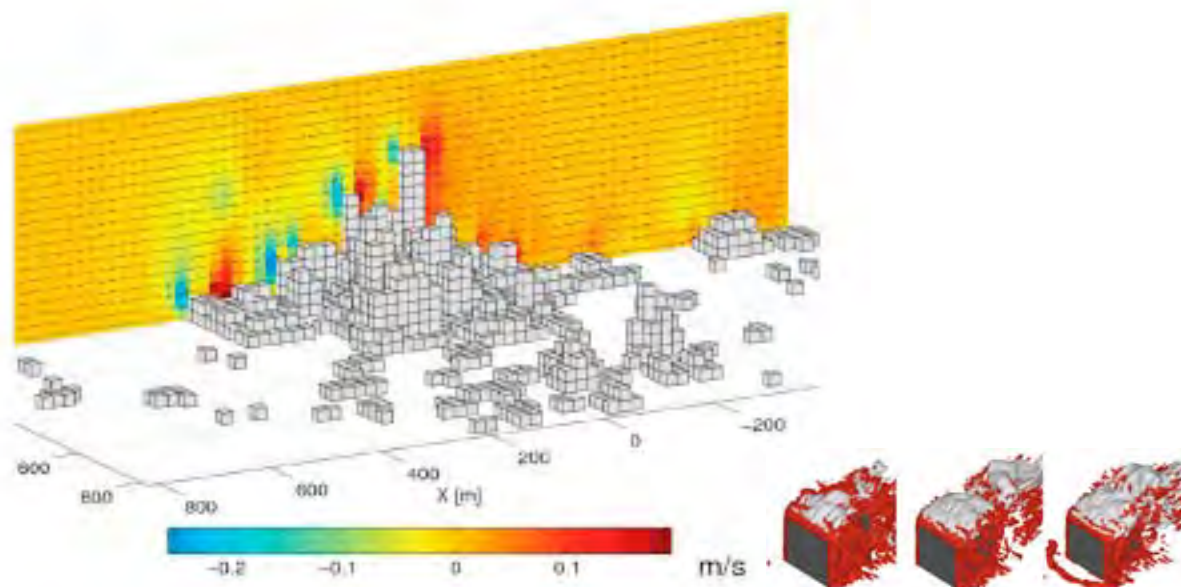
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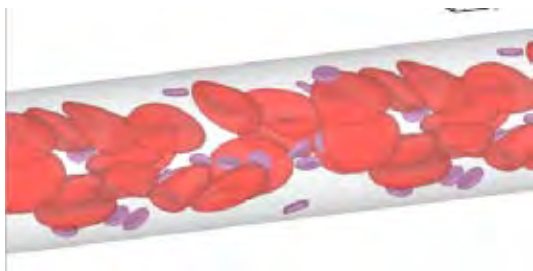
"Our investment in medical S&T provides the basis for maintaining the physical and mental health of Soldiers as well as enhancing their performance. ... For Battlefield Trauma Management, a primary focus is to address the single greatest potentially preventable cause of combat — internal hemorrhage. This requires an integrated approach which includes controlling bleeding, replacement of lost fluid volume, cells, and clotting capability, and providing fluids and adjuncts to maintain adequate delivery of oxygen to critical tissues."
— Dr. Thomas H. Killion
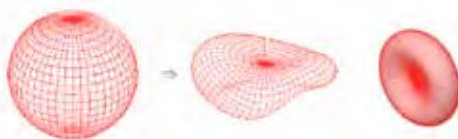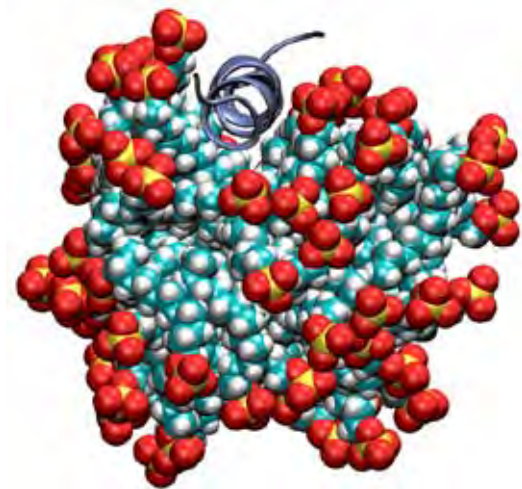
Many phenomena that happen on the scale of molecules, viruses, and bacteria can produce significant effects at the scale of a human body, a building, or an entire city. Material and biological systems at nano- and microscales play an increasing role in Army scientific and engineering endeavors. This research not only draws on existing knowledge of fluid dynamics, molecular modeling, and materials engineering—it requires new insights into the unique behaviors of molecules and particles at very small scales.

Computer simulation is ideally suited to setting up realistic scenarios and studying the interplay of many factors. High performance computing can be used to design antibacterial and antiviral agents "from the atoms up"; to model blood flow at the microcirculation level; or to simulate the complex interplay of topological and meteorological factors affecting the spread of a contaminant plume over a city. The speed and capacity of massively parallel computers are key to simulating real-world phenomena on scales ranging from nanometers to city neighborhoods.

AHPCRC research in this area deals with detecting, protecting against, and responding to harmful biological agents (natural and engineered), as well as developing better ways to deliver blood additives and treat traumatic injuries.

Clockwise from top left: Air flow velocity map for downtown Oklahoma City, turbulent flow over a 3D obstacle (M.Z. Jacobson, G. Iaccarino, Stanford). Cecropin peptide penetrates a micelle surrogate for a bacterial membrane structure (E. Darve, Stanford). Calculated virus protein structure includes side-chain details (J. He, NMSU). Red blood cells push platelets toward capillary walls (E. Shaqfeh, Stanford).

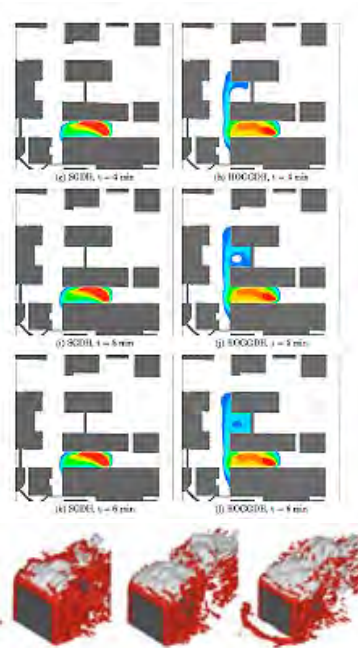# Project 2–1: Dispersion of Biowarfare Agents in Attack Zones

Principal Investigators: Gianluca Iaccarino, Eric Shaqfeh, and Mark Z. Jacobson (Stanford University)

Planning an emergency response to the release of airborne toxins requires an understanding of the interactions among the initial contaminant plume, the terrain topology and buildings, weather conditions, and photochemical reactions in the atmosphere, —all these influence the size and location of the evacuated area and the duration of the event. Real-world field studies for emergency response planning are expensive and require complex planning and execution. Thus, high-performance computer simulation can play a key role in improving our ability to plan emergency responses.

Computer simulations integrate real-world information from many sources to construct predictions and "what-if" scenarios. Simulations factor in numerous parameters and variables along with model agent behavior over a sufficiently long time span to produce useful results. Massively parallel codes and HPC facilities provide the computing resources necessary to run realistic simulations of this nature. AHPCRC simulations of downtown Chicago have shown significant differences in the

Top: Contaminant plume spread simulation for downtown Oklahoma City using two different turbulent methods (left and right columns) at 4, 5, and 6 minutes. *Bottom:* Simulation of turbulent flow over a 3D obstacle (R. Rossi, D. Philips, G. Iaccarino, Stanford)

dispersion of biological warfare agents as a function of local topographical features, such as rivers and buildings. More recent simulations replicated the conditions during a 2003 planned release field study in Oklahoma City.

The AHPCRC simulations use one modeling method for the neighborhood, city, and global levels, and another for the immediate vicinity of the release, where rough terrain and building wakes play fundamental roles. Information is passed back and forth between the two methods to improve the fidelity of the predictions.
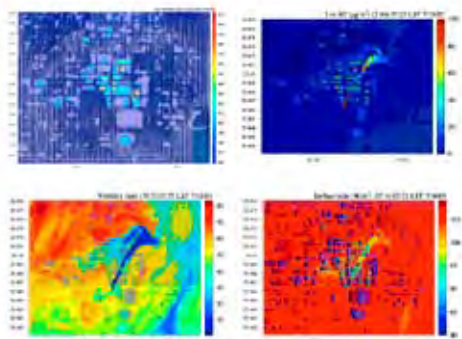
Clockwise from top left: Simulated wind velocity, tracer concentration, solar power, visibility over Oklahoma City, 12m resolution. (M.Z. Jacobson, Stanford).

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Health Protection

Project 2–2: Micro- and Nano-fluidic Simulations for BWA Sensing and Blood Additive Development

Principal Investigators: Eric Shaqfeh and Eric Darve (Stanford University)

Microfluidics is the study of suspensions and solutions flowing through channels barely large enough for particles to pass. Microfluidic models provide valuable insights on designing portable devices for sensing and identifying biological warfare agents (BWAs), as well as for developing medical treatments for traumatic injuries.

Many lab-on-a-chip devices contain fluid channels just wide enough to accommodate a few large molecules such as DNA. Some molecular "bar code" devices contain capillaries that force submicron objects to pass through a channel in single file. Human capillaries can be narrower than a single red blood cell, forcing cells to deform in order to squeeze through.

When the width of a channel is roughly the same size as the particles flowing through it, conventional fluid dynamics principles no longer apply. Essentially all of the particles are in contact with the walls of the channel, leaving no area of free flow in the center. Particle shapes and channel dimensions and geometry take on increasing importance. Irregularly-shaped or elongated particles can form snags and obstructions. Particles adhering to the channel walls (blood clots, for instance) affect the characteristics of the flow. If the particles interact electrostatically with the channel walls or with each other, this adds additional complexity.
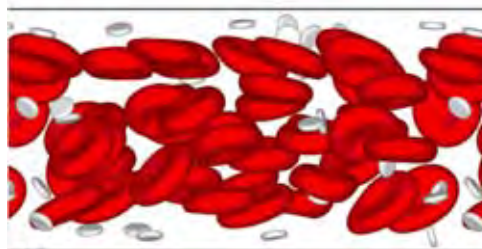
Army medical researchers are especially interested in developing methods for reconstituting freeze-dried human blood platelets in the field for the treatment of serious wounds. Current techniques for freeze-drying require a multi-step procedure involving chemical fixers to keep the platelets from agglomerating, and reconstituted platelets are not as effective as platelets in their native state.

Recently, AHPCRC researchers at Stanford completed a set of computer simulations of platelet and red blood cell microcirculation behaviors. These simulations show that, at the high shear rates typical for small vessels, red blood cells gradually move toward the center of the blood vessel, forcing the platelets toward the vessel walls. This behavior replicates observations from life, where platelets concentrate near the blood vessel walls, ready to trigger the sequence of events that stops the bleeding when a blood vessel is damaged.
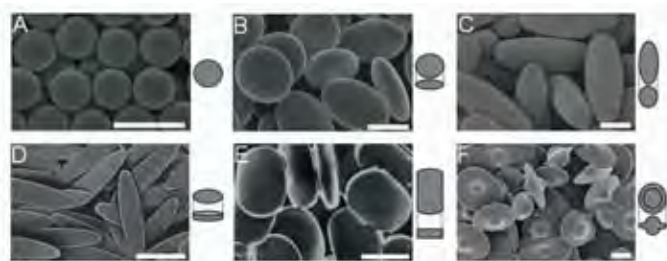
Top: Simulation of red blood cells and platelets in a capillary. (E. Shaqfeh, Stanford).
Bottom: Electron micrograph of laboratory test particles for drug delivery. (S. Mitragotri, UCSB).

Project 2–3: Design of Antimicrobial Peptides for Nano-Engineered Active Coatings

Principal Investigator: Eric Darve (Stanford University)

Microbes—naturally occurring or intentionally introduced—can cause debilitating disease outbreaks, food spoilage, and corrosion. Antimicrobial coatings are being developed to protect many types of surfaces that are at risk from microbial contamination—kitchen countertops, protective apparel, and ship hulls, to name a few. These coatings help prevent the transmission of harmful microbes among items coming in contact with a coated surface, but they also protect the underlying structures from damage due to mold, fungus, bacteria, and the substances that they produce.

AHPCRC research in this area focuses on mathematical methods and numerical algorithms that describe interactions between antimicrobial peptides—the building blocks for protein molecules—and bacterial cell membranes. Cecropin, a well-characterized antimicrobial peptide produced by some insects, is being used as a test case.

Computer simulations show the folding and unfolding of cecropin molecules in water and at the interface between water and a cell membrane. These simulations will assist in understanding the mechanisms by which antimicrobial peptides contact, penetrate, and puncture bacterial cell membranes without harming the cells of humans and animals.

The Stanford group has produced computational models of the interaction of Cecropin with micelles (molecular clusters that behave in a similar fashion to cell membranes). They are also designing computational models that can be compared with flat-surface binding experiments being conducted in Army laboratories. This will assist them in simulating interactions between antimicrobial peptides and the lipopolysaccharides (LPS) that form actual cell membranes. Successful models will assist the intentional design of potent broad-spectrum antimicrobial agents.
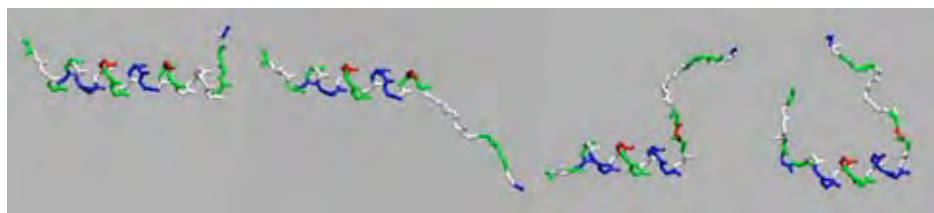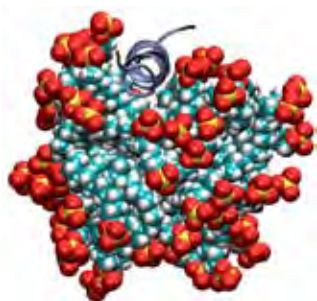

Top: Molecular structure of cecropin peptide. *Above:* Time sequence, cecropin molecular backbone unfolding in water. *Left:* Cecropin helix penetrates a micelle that acts as a model of a bacterial cell membrane. (Graphics this page: E. Darve, Stanford)

Project 2–4: Protein Structure Prediction for Virus Particles

Principal Investigator: Enrico Pontelli (New Mexico State University)

Viruses, one category of biological warfare agents, are essentially packets of genetic material encased in protein shells. The structures of these proteins play an important role in the functionality of a virus, and also provide a means of identifying and designing vaccines against specific viruses. Viruses mutate rapidly and can be genetically engineered to resist existing vaccines. Protein structure prediction methods can point to likely adaptations of known viruses and guide efforts to combat the new forms. These methods are computationally intensive and require advanced visualization tools to be effective—making them ideal candidates for high performance computing.
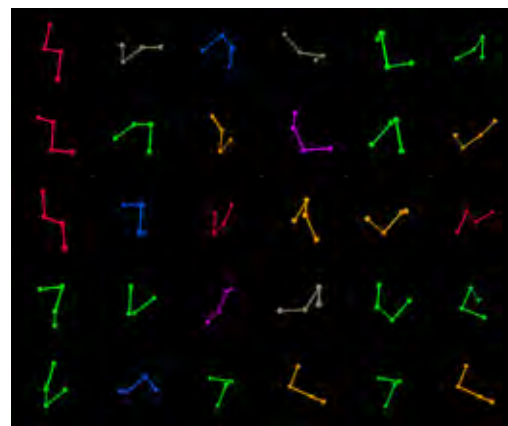
AHPCRC researchers are developing a constraint-based ab initio protein structure predictor—a computational method that builds protein structures "from the ground up" using known constraints on the types of structures that proteins can take on. The NMSU group assembles simplified protein chain models into structure fragments using a library of possible conformations taken from the Protein Data Bank (PDB), a repository of known protein structures. Because of the large number of these conformations and the even larger number of possible structure fragment combinations, the NMSU group is working on parallel search capabilities using cluster computing, graphics processing units (GPUs), and multicore computational environments.

Possible configurations must be ranked according to the likelihood of their occurrence. The most energetically stable forms are also the most likely to occur. The NMSU group has added capabilities for representing molecular side chains and for restricting the number of configurations considered during a search using the composition of fragments collected from the PDB.

Intentionally engineered virus structures are one promising avenue of application for computational structure prediction research. Because viruses are naturally self-replicating nanoparticles, they have potential use as drug delivery devices. A thorough understanding of virus structures and their functions is vital to ensuring that such engineered viruses are safe and effective.

Top: Clustered conformations for AAAA fragments. Each color has a representative and a frequency count. (E. Pontelli, NMSU) *Bottom:* Protein secondary structure with side chains. (J. He, NMSU)
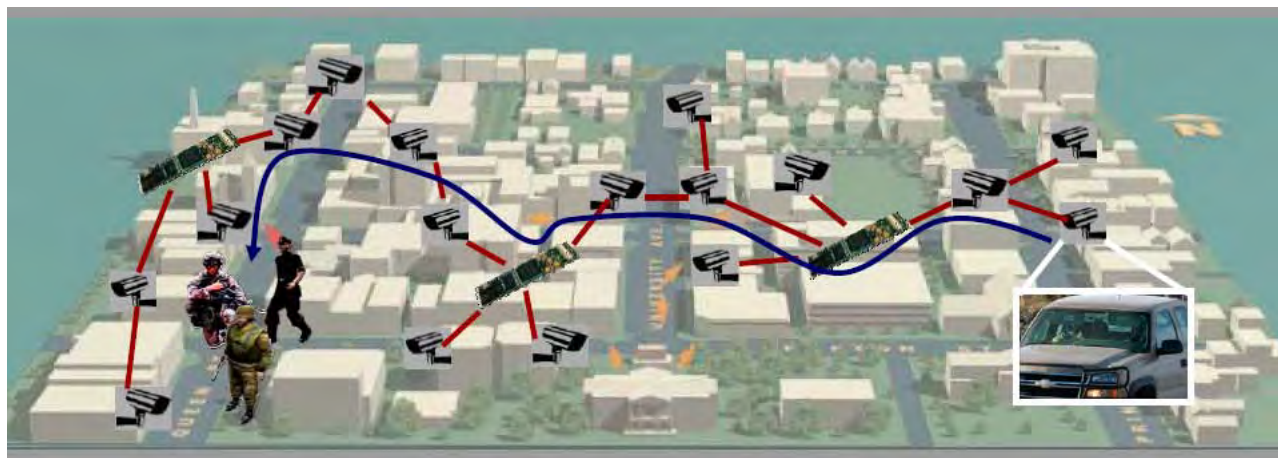
Battle Command

The modern warfighter can no longer expect to engage an easily recognizable enemy on a clearly defined battlefield. Hostile forces are increasingly difficult to distinguish from civilians, targets are hard to identify, and intelligence information is rarely clear and unambiguous.

To meet these challenges, AHPCRC researchers are designing wireless sensor and communication networks that provide detailed, accurate, and reliable information-gathering capabilities and decision support for soldiers in the field. One area of focus is the gathering and in-network processing of data to provide end users with relevant, meaningful information in the shortest time possible. High performance computers, at centralized locations or built into the network itself, integrate inputs from many sources and provide context and visualization to aid in interpretation and decision making.

The networks themselves are a second area of interest. Sensors and communications links must be arranged and connected so as to provide reliable coverage over the area of interest, high throughput, and defense against hostile interference or eavesdropping. Often, such networks must be constructed quickly in a hostile urban environment, and they must maintain contact with mobile users moving in unpredictable patterns. High performance computing enables simulations of complex network configurations and the ability to test many scenarios before trying them out in the field.

Mixed Network Associations

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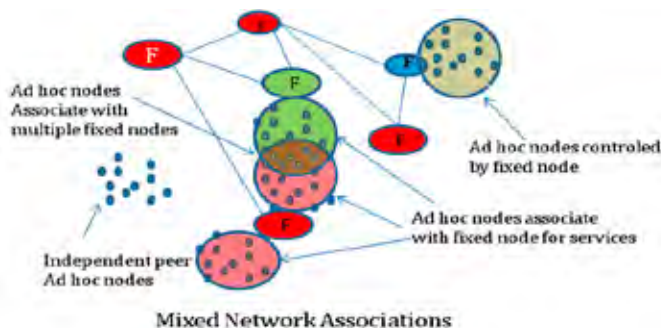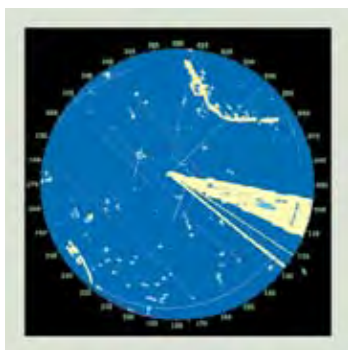
"Army science and technology is working on advancements in information transport and on enabling improved collaboration for the Warfighter. For information transport at the tactical level, Army science and technology is investing in lower cost, more capable satellite communications antennas for current and planned satellite constellations. Additionally, science and technology is developing the software application for existing radios to better utilize the limited RF spectrum in military operations. Research and development is underway to more seamlessly share information across functional domains. This will allow more timely interaction and sharing of information across intelligence, planning and battle operations."
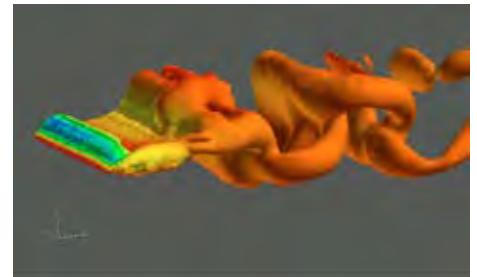*— Dr. Thomas H. Killion*

Micro aerial vehicles (MAVs) are tiny, stealthy, affordable aircraft that serve as the soldier's eyes, ears, and nose in hazardous or inaccessible areas, or in situations that require round-the-clock surveillance. High performance computing helps MAV designers understand the aerodynamic properties of these vehicles, leading to designs that provide the greatest lift and thrust for the least amount of energy input. Computer simulation allows designers to try out numerous mechanical and material configurations to see which ones work best.

High performance computing aids in designing birdlike flapping and twisting wings. These allow micro aerial vehicles to maneuver in tight spaces and stay on course despite unpredictable gusts and air currents. Simulations show how real birds generate lift and propulsion, and quantify the energy needed for flight.

Clockwise from top left: Quality of Service (QoS) routing assigns and guarantees level-of-service priorities for various users (L. Guibas, Stanford). Virtual street scene assists in designing and integrating data from camera networks (L. Guibas, Stanford). 3D simulation of flapping wing shows vortex formation during flight (A. Jameson, Stanford). Mechanical MAV model validates computational results (M. Wei, NMSU). Mobile ad hoc network components (R. Dean, Morgan State). Radar scan with jamming in one sector (Wikimedia Commons).

Project 1–3: Multidisciplinary Parametric Modeling and Lift/Drag Quantification and Optimization

Principal Investigators: Antony Jameson (Stanford University)

Small, inexpensive flying drones can serve as the soldier's eyes, ears, and nose in situations that are hazardous or that require 24 x 7 attention. Small flying vehicles face challenges, such as air turbulence and viscosity properties, that larger flyers do not. Bird-sized micro-aerial vehicles (MAV) have roughly 10% the lift to drag ratio of larger aircraft, which limits their range and endurance.

Birds and insects provide effective design examples, but imitating these flyers is a complicated task, involving flexible wing structures, complex wing motions, and unsteady viscous flow. Unlike their natural counterparts, drone vehicles cannot spend most of their time in a search for fuel. Drone vehicle wings must achieve the most lift and propulsion with the least expenditure of energy, so that the drones can carry their load of sensors, communications devices, and fuel.

Computing one three-dimensional unsteady viscous flow solution can require on the order of 10 CPU hours, and flapping wing optimizations require thousands to tens of thousands of such solutions. Creating realistic models of deformable three-dimensional wings in periodic motion requires the use of massively parallel computational systems and software that is optimized to make the most efficient use of the available hardware.
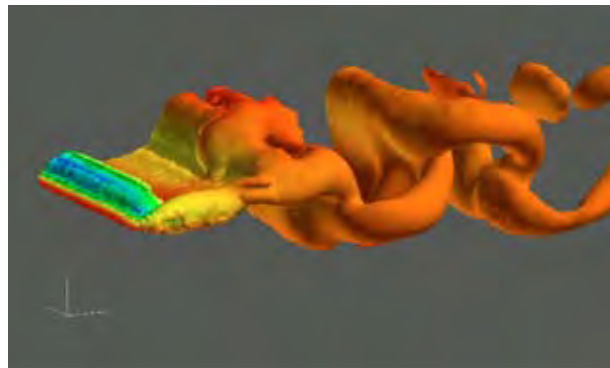
AHPCRC researchers are using massively parallel HPC simulations to create wing models that maximize lift and minimize drag. These simulations have provided insights into the propulsive efficiency of various pitching and plunging motions of three-dimensional simulated wings. Large-scale three-dimensional turbulent flow simulations are being used to verify the fast two-dimensional shape optimization process for MAV airfoils.

The Stanford group is collaborating with the group in Project 1–7 to implement optimization algorithms into their calculations. New solvers purpose-built for flapping wing optimization have been developed to meet the demands for accurate flow physics and mesh motion. These solvers have been put into use for optimization of the motion of a 2D airfoil and a 3D wing. Software tools now exists to perform flapping optimizations using a wide range of motion parameterizations and wing geometries.
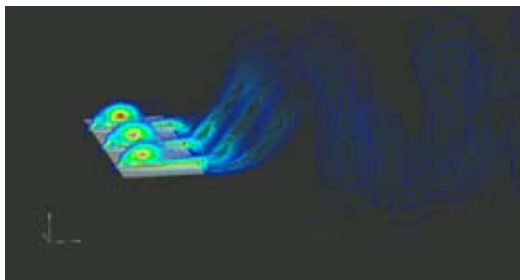
Top: Isovorticity contours for a flapping wing.
Bottom: Spanwise flow patterns for a flapping wing.
(Graphics this page: A. Jameson, Stanford)

Project 1–4: Flapping and Twisting Aeroelastic Wings for Propulsion

Principal Investigators: Charbel Farhat (Stanford University); Mingjun Wei, Banavara Shashikanth, Fangjun Shu (New Mexico State University)

Birds and insects use complex flapping and twisting wing motions to maneuver, hover, avoid obstacles, and maintain or regain their equilibrium in shifting and unpredictable wind currents. Flocks of birds travel in formation and insects form unstructured swarms using rudimentary communications. Parameterizing and simulating bird and insect behaviors will be instrumental in developing small, lightweight, sturdy unmanned aerial vehicles for use in sensing, surveillance, and wireless communications.

HPC simulations examine plunging, pitching, and twisting motions of aeroelastic wings, to optimize the amplitudes and frequencies of flapping and twisting motions for the maximum amount of thrust.

AHPCRC researchers at Stanford and NMSU are working on two separate, but related, aspects of the wing problem. Several methods of calculation are being adapted, extended, and validated for this purpose.

The Stanford group is upgrading the massively parallel AERO computational fluid dynamics code to enable it to simulate the flapping and twisting of aeroelastic wings using provably superior computational algorithms. They have devoted considerable effort to modeling the interface between the solid wing and the fluid atmosphere through which it moves. They now have modeling capabilities for inviscid and laminar flows, as well as linear and nonlinear structural dynamics. The group is working on hooking their turbulence models into the software, which performs scalably on massively parallel systems.

Ornithopter in a wind tunnel.
(M. Wei, NMSU)

The NMSU group combines computational, theoretical, and experimental approaches to gain an understanding of fluid–structure interaction, leading to optimum thrust, lift, drag configurations and conditions for flapping wing objects. This is necessary for MAV development, design and deployment. They are validating their computational results against mechanical wing and bird models deployed in a water tank and a wind tunnel. An oil tank setup is under development to extend the range of viscosities and density ratios that can be examined.

Computational fluid dynamics model, surface view.
(C. Farhat, Stanford)

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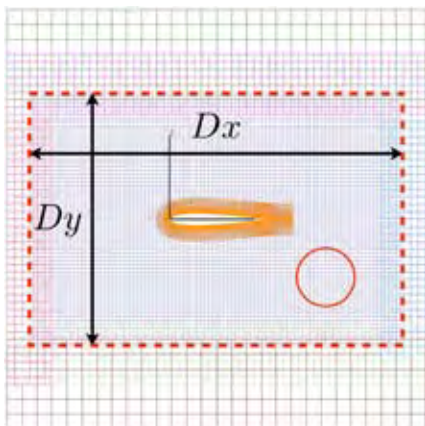www.ahpcrc.org
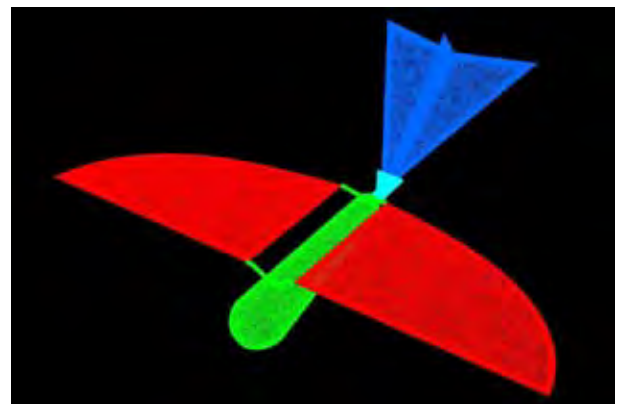
Project 1–5: Numerical Simulation of Flapping Flows

Principal Investigators: Terry Holst, Thomas Pulliam, Piyush Mehrotra
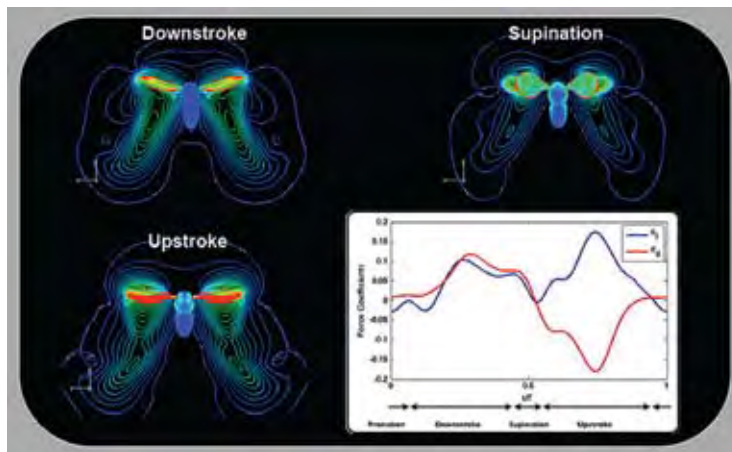(NASA Ames Research Center)

Simulating the behavior of flapping-wing micro-aerial vehicles (MAVs) is computationally expensive. Identifying bottlenecks in the computational process and tracking the accuracy and efficiency of various computational fluid dynamics (CFD) packages is a necessary factor in making these codes readily available for use by designers and engineers.

AHPCRC researchers at NASA Ames are formalizing two-dimensional plunging airfoil studies, establishing correlations with experiments and other simulation efforts; developing guidelines for grid resolution, spatial accuracy, and time accuracy; and studying the performance of the code for the moving grid case with various numbers of message passing interface (MPI) groups and open multiprocessing (OpenMP) threads, paying particular attention to the performance of the portions of the code that deal with grid motion.

Investigations of NASA's OVERFLOW code have shown that the geometric operations required by moving grid calculations do not pose a computational bottleneck under the conditions studied. An analysis of Stanford's AERO-F code

Trajectory and load history for flapping fruit fly wings. See also the related figure, next page. (Graphics this page: T. Holst, NASA Ames)

showed four functions that consume most of the computational time and are possible targets for optimization work.

Preliminary two-dimensional airfoil analyses have been performed, using OVERFLOW2.1 on the NASA Pleiades system (40,000 cores) to find solutions for a rigid NACA 0012 airfoil undergoing generalized pitching and plunging motion.

A new grid movement technique has been implemented and validated to model correctly a two-dimensional combined pitching and plunging motion. Grid refinement studies are being done to establish the optimal domain and grid sizing. These studies are guiding selection of the optimal temporal solution parameters, a key requirement to limit the computational cost, especially for optimization, which will require large numbers of flow solutions.

Setting up the grid parameters for the plunging wing model.

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Battle Command

Project 1–7: Advanced Optimization Algorithms and Software

Principal Investigators: Walter Murray and Michael Saunders
(Stanford University)

Optimization, a means of finding the most efficient way of solving complex mathematical problems, is a vital part of most branches of computational science and engineering. General-purpose optimization packages are constantly finding new applications in such areas as aerospace, economics, geophysics, and manufacturing. Shape optimization and trajectory optimization for aircraft and spacecraft are important to all branches of the Department of Defense.
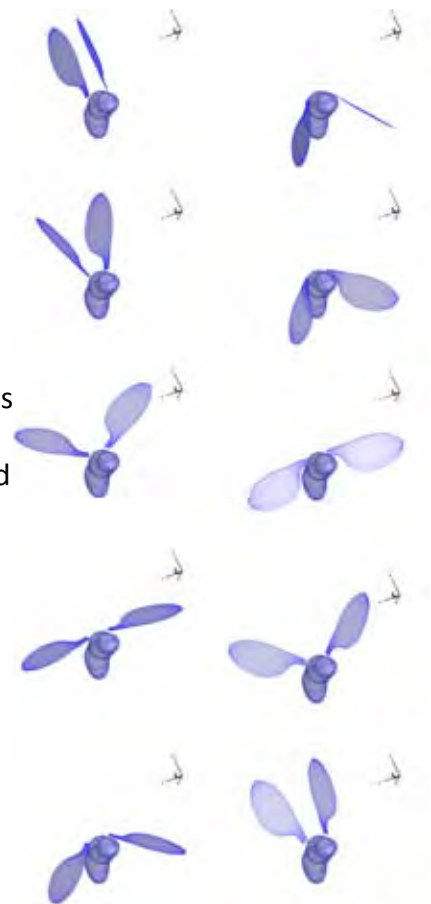
AHPCRC researchers at Stanford are enhancing existing computational packages by incorporating high performance computing techniques such as parallel linear-system solvers, and to assist other AHPCRC projects in need of optimization techniques.

A major focus of this research addresses solving partial differential equation (PDE)-constrained optimization problems such as those arising in the design of micro-aerial vehicles (MAVs) capable of serving as airborne video or sensor platforms. One such problem is the determination of optimal wing shapes and motions. Work in progress involves coupling the PDE-solver AERO-F and the large-scale optimization solvers SNOPT and SQOPT. Each of these programs is already in widespread use, and enabling them to work together is anticipated to provide even greater problem-solving capabilities.

The group is making significant improvements to SNOPT, reducing the number of required objective function evaluations, and employing more efficient hot starts. The goal is to link SNOPT with PDE software running on multiple processors. New, more efficient, versions of the AERO-F and the multigrid solver UFLO103 will be developed for use with many types of codes.

High performance optimization tools facilitate wing design for micro-aerial vehicles. (T. Holst, NASA Ames)

In addition, the Stanford group is developing a stochastic matrix-free scaling algorithm for matrices. Also in the works is a version of the active-set convex quadratic programming (QP) solver QPBLUR that runs in MATLAB and FORTRAN95 for the solution of large QP problems. The Stanford group also performs basic research in optimization and linear algebra, especially for the solution of large and intractable problems.

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Project 2–6: Multiscale Modeling of Materials
## Principal Investigator: Eric Darve (Stanford University)

Building a single radar system for multiple tasks, such as surface and air detection, tracking, and missile uplinking, requires phased antenna arrays. The radiation patterns in these arrays can be enhanced or suppressed in desired directions. Phased antenna arrays can be significantly smaller than their conventional counterparts, and they can encompass a field of view approaching 120°. Key to the development of such technologies are ferroelectric materials, whose dielectric constants can be altered to specific values by the application of an electric field. Barium titanate ($BaTiO_3$ or BTO) is one of the best-characterized ferroelectric materials.

Existing computational force fields are sufficient to model BTO crystals using molecular dynamics (MD) methods, including accounting for dipole charge interactions within a crystal. However, it is difficult to construct accurate models for the transitions among the four configurations (phases, represented at left) that the BTO crystal lattice is known to assume using available force fields and parameterizations. In addition, no force field is currently capable of modeling vacancy (defect) diffusion in the crystal, an important factor in modeling material behavior under real-world conditions.
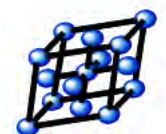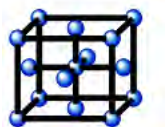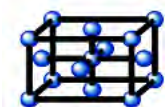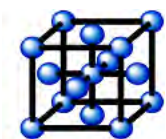
Barium titanate phases.
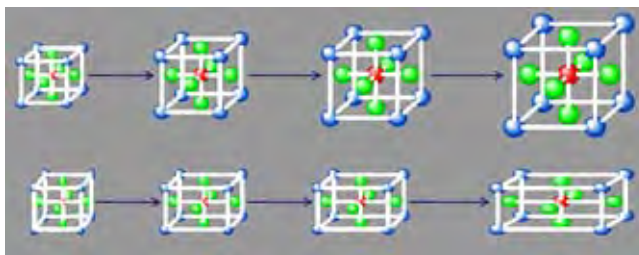
Deforming crystals of barium titanate changes their electrical properties. (Graphics this page: E. Darve, Stanford)

AHPCRC researchers at Stanford have created a unique set of tools to address these challenges, based on genetic algorithms. By tailoring the force field model specifically for BTO, the behavior of the crystal can modeled with a high degree of fidelity under a diverse range of physical and electrical loading conditions.

Density functional theory analysis provides various energy configuration curves that the genetic algorithm consequently uses as a reference database. The genetic algorithm evaluates potentials using various parameter sets, and the resulting difference between the energy produced from the potential and that of the reference database is used to establish the "fitness" of the given parameter set. Members of a population are consequently combined to create "offspring" with increased fitness. As the genetic algorithm produces generation after generation, the algorithm strives to produce parameter sets with ever-greater fidelity to the quantum energy calculations. Further refinements to the technique include coupling a steepest-descent optimization method to the genetic algorithm.

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Project 3–1: Information Aggregation and Diffusion Under Mobility

Principal Investigator: Leonidas Guibas (Stanford University)

Mobile ad hoc communications and sensor networks must provide timely, usable information to many mobile authorized users. In-network HPC assets can aggregate streams of raw data and perform in-network analysis in order to deliver useful, highly specific information to the users. Off-line HPC resources can be used for network planning protocol optimization, and sensor data analysis, allowing customization and adaptation of the network resulting in more efficient use of power and bandwidth.

Image webs annotate and identify common features from multiple image sources. (Graphics this page: L. Guibas, Stanford)

AHPCRC researchers analyze user mobility and communication patterns to develop better algorithms and protocols for delivering information to mobile users within the network. This work is aimed at improving network layouts, determining the number of nodes and their placement, adapting protocol parameters, and establishing methods for delivering data efficiently.

Image webs, a method for annotating and discovering interconnections among hundreds of thousands of sensor-acquired images, gives insights into tracking people and vehicles moving within a sensor network. Image annotations and other symbolic information can be propagated and shared through image web links. These large sig-

Image region graph provides a simplified representation of the arrangements of objects in an image.
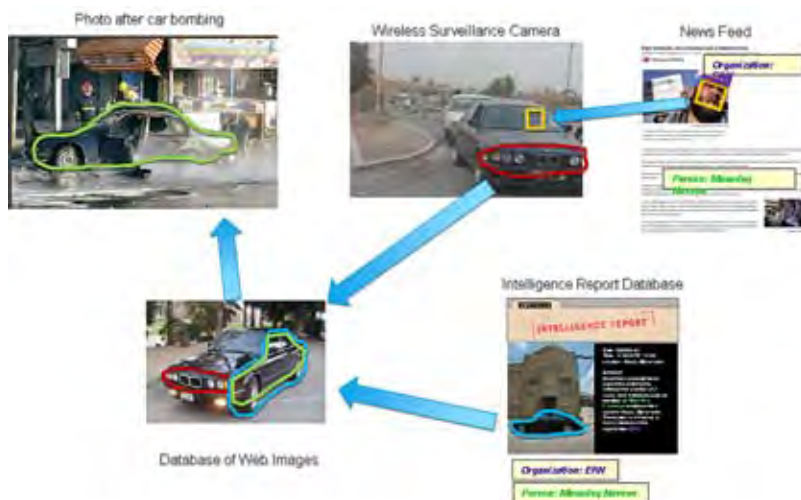
nal graphs can also provide a means of orienting and guiding robotic vehicles, using recognizable features of the environment to establish location and direction. Image webs greatly benefit from HPC capabilities, because they require significant computational resources to identify and correlate image features, and to fuse signal data into a holistic scene understanding.

Because communication in a networked environment requires even more resources than computation, relevant image features are extracted, annotated, and prioritized at the site of each camera, then relayed to the network.

A small testbed network implemented at Stanford University is used to develop the concepts and methods produced by the computational studies. Testing is done using miniature camera and wireless sensor nodes (Citric and TelosB motes), small Linux computers (Gumstix), WiFi camera units, Droid phones, and iRobot mobile nodes.

Project 3–2: Scalable Design Methods for Topology Aware Networks

Principal Investigator: Amin Saberi (Stanford University)

A complex military network must be well-connected and robust in a highly mobile and dynamic environment. This AHPCRC project focuses on characterizing the structural properties of the underlying network that affect the performance and scalability of communication protocols. Algebraic graph theory is used to define metrics that characterize the global connectivity status of the network and identify the "critical areas" such as holes or narrow bridges. These metrics can be computed by low-overhead, scalable, and local message passing algorithms.

Such an understanding of network structure has several applications at the information dissemination level: a global understanding of the network topology allows local "greedy" methods for information discovery and brokerage to work effectively and in a load-balanced fashion. This structural understanding also helps with the implementation of mathematical methods by helping to find the correct boundary conditions, establishing rendezvous points, and other factors.

AHPCRC researchers at Stanford aim to provide appropriate and easily computable metrics for the network connectivity. This will enable network clients to determine whether a given network configuration provides adequate global connectivity, without knowing the whole network.
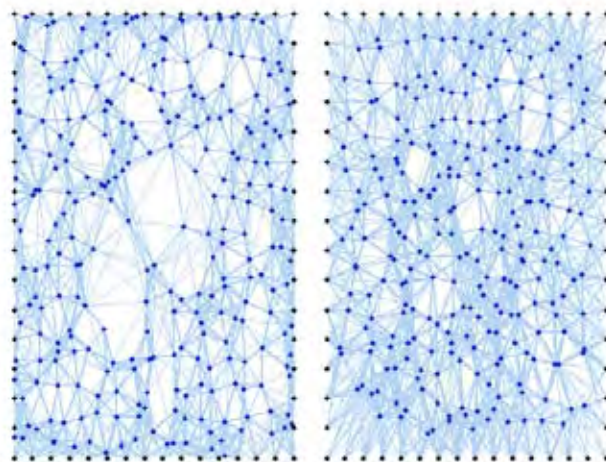
The distribution of nodes in a network is reconfigured to achieve optimum connectivity using a low-overhead distributed algorithm developed based on algebraic and graph theoretic methods. (A. Saberi, Stanford)

The Stanford group is also working on developing novel local and decentralized schemes for enhancing network connectivity. Part of the theoretical work done in this project makes a deep contribution in approximation algorithms and spectral graph theory. In particular, the subgraph sparsification technique developed for the project can be applied much more widely (for example, solving linear systems).

# Project 3–3: Secure Sensor Data Dissemination and Aggregation
Principal Investigator: Hong Huang (New Mexico State University)

Military sensor nets must be designed such that the network cannot be co-opted or used effectively by an adversary, but security constraints must be balanced with the need for fast, efficient in-network processing. Optimizing the complex tradeoffs between processing, security, communication bandwidth, and power consumption in complex urban settings will push the frontier of high performance computing.

Of particular interest is the ability of a distributed jamming network (DJN) to jam signals in all or part of a sensor or communications network. Swarms of tiny, low-powered radio signal emitters released within a target network can effectively disrupt signal transmission. Recent advances in nanotube radios and micro-electro-mechanical systems (MEMS) have reduced the size of these signal emitters to the dimensions of a speck of dust. A jamming "dust cloud" is effective because the large number of emitters provides redundancy, low power requirements reduce self-interference effects, and the tiny size and low power emission of the particles makes them difficult to detect.
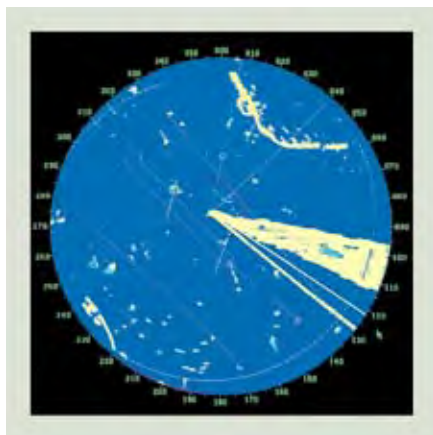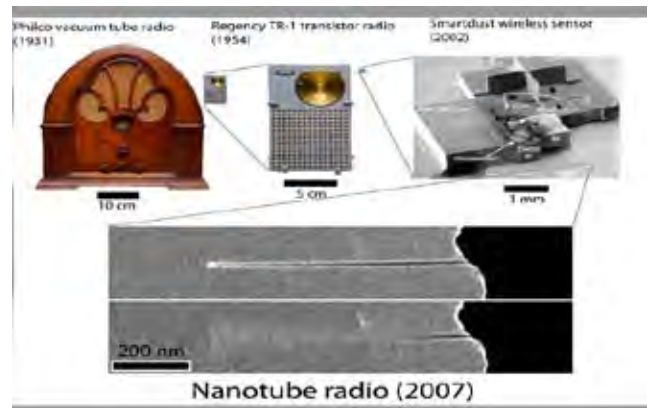
A history of radio miniaturization. (H. Huang, NMSU)

Radar scan with jamming in one sector. (Wikimedia Commons)

A DJN can be deployed to disrupt the communications of an adversary or radio triggering mechanisms on explosive devices. The DJN requires little power, and thus does not disrupt friendly force communications.

AHPCRC researchers at NMSU are investigating phase transitions that a DJN produces in a target network, and they are determining critical values for the number and power of jammers within a DJN. They are also studying the effects of node mobility and the topology of the DJN on jamming effectiveness. They have examined the effects of jamming at null frequencies, where a low level of network congestion can produce a significant collapse of performance.

Current research focuses on the relationship between network capacity and network size in the presence of a DJN, and coordinated and adaptive jamming effects. They are also developing counter-measures against DJNs. This research relies on accurate HPC simulations of large-scale networks to model network configurations and responses under numerous scenarios.

Project 3–4: Robust Wireless Communications in Complex Environments

Principal Investigators: Richard Dean, Gregory Wilkins, and Yacob Astatke (Morgan State University)

A warfighter's ability to function in a complex computational battlefield environment is complicated by the mix of tactical and strategic assets that are constantly changing as he moves through the environment. Much is known today about standalone wireless mobile ad hoc networks (MANET) and much is known about fixed network resources. Little is known, however, about how these resources can be dynamically mixed to support the mission.

AHPCRC researchers are focusing on the development of a network strategy that mixes fixed and mobile networks to the overall performance advantage of both. This work draws on multistage clustering techniques that have the potential for near optimum performance with an inherently efficient computational scheme.

The Mixed Network solution developed at Morgan State University addresses the performance of fixed telemetry ground networks with associated mobile nodes within the range of the ground station and disconnected mobile nodes that are over the horizon and operate as a MANET. A multistage clustering scheme can organize all the
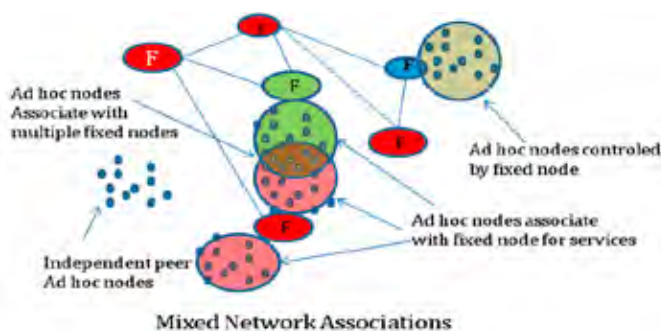
Mobile ad hoc network components (Graphics this page: R. Dean, Morgan State University)

nodes into clusters that are in either a ground-based cluster or in one of several ad hoc clusters. Such a scheme can jointly enhance the performance of all the nodes using a distance measure that includes location, Quality of Service (QoS) performance, and interference management of these nodes in static and dynamic environments.

Under the AHPCRC program, research focuses on extending the current Mixed Network strategy to a larger framework and exploring the computation and performance features. Such a strategy would move from a single fixed network with multiple ad hoc networks to a multiplicity of fixed networks with a multiplicity of associated ad hoc networks. Nodes could gravitate toward competing fixed network elements on the basis of service and performance. "Market behavior" captured in distance measures would adapt network traffic to support best-value services.
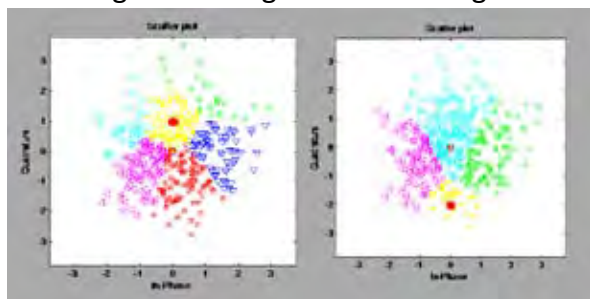

Single-stage clustering with a mobile base station (red dot).

Project 4–7: Evaluating Heterogeneous High Performance Computing for Use in Field-Deployable Systems

Principal Investigator: Jeanine Cook (New Mexico State University)

The emergence of heterogeneous high performance computing (HHPC) systems and the increased processing capability that these systems enable has enhanced the advantages of using them in field situations. The computational power, the decreased size, and the focus on reduced power consumption enables the integration of CPUs and accelerators (GPUs, FPGAs, solid state devices) into small systems with enough compute capability to execute critical military applications in the field, in real or near-real time.

To determine the appropriate architecture of a field-deployable HHPC system, constraints in terms of application performance, computational precision, power dissipation, size, and weight must be considered. Since many military-related applications depend on real-time production of results, operating system performance with respect to both execution time and power dissipation is also important.
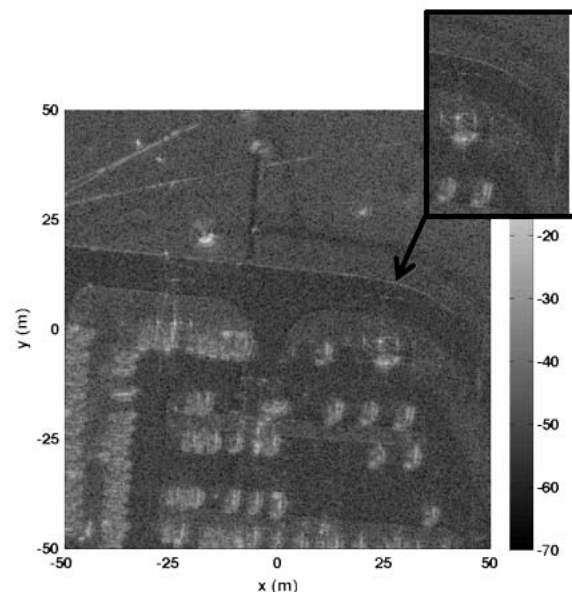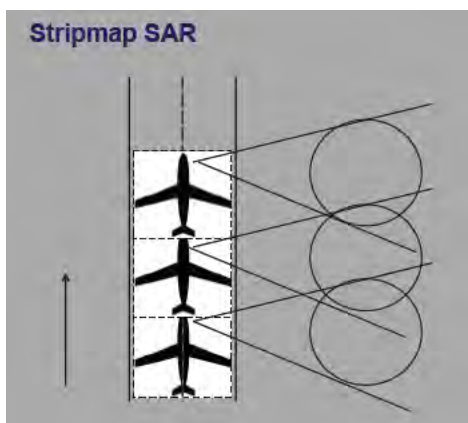
Synthetic aperture radar (SAR) digitally combines multiple images to produce a single image having the same high resolution as a much larger radar antenna. (Graphics this page: P. Teller, UTEP, top; J. Cook, NMSU, bottom).

AHPCRC researchers at NMSU are investigating the capability of HHPC and how it can be used in field-deployable systems to aid soldiers in real-time decision-making and strategic analysis in battlefield situations. To design such a system, researchers are studying the performance of relevant applications on various compute technologies, including processing the data-intensive image streams produced by synthetic aperture radar (SAR). The researchers foresee the extension of the capabilities they develop here to other areas, including situational awareness and strategic decision-making applications.


Stripmap SAR

A moving aircraft takes a series of radar images that are processed into a single image like the one above.

Project 3–5: Mobile Brain–Machine Interface for Integrated Information–Social/Cognitive Network Operations

Principal Investigator: Kwong T. Ng (New Mexico State University)

An information network must have precise knowledge of the social/cognitive network's mental state, so it will provide information suited to human cognitive capabilities in collaborative operations. This project will use a brain-machine interface (BMI) as a sensor of human cognition, and use it to extract quantitative neural signatures that represent the state of the social/cognitive network. The servers in the information network can dynamically query humans and request sensor data sent through the battlespace mobile communication network to designated processors for neural signature extraction. The human neural signatures can then be used collectively to perform communication, command and control functions.

(New project, 2010)
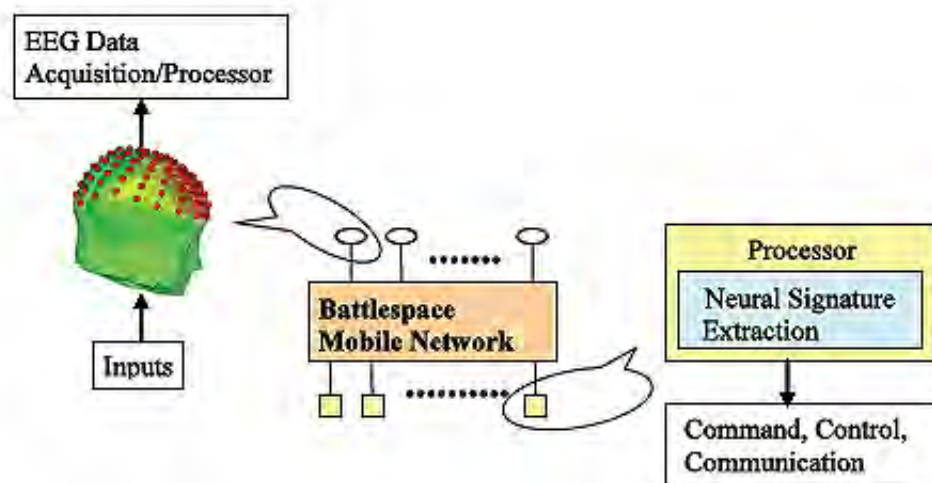
Mobile brain–machine interfaces connected to the battlespace network. (K.T. Ng, NMSU)

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Project 3–6: Modeling Socio-Cultural Processes in Network Centric Environments

Principal Investigator: Eunice E. Santos (University of Texas at El Paso)

The Army's modernization plans call for network integration of manned and unmanned vehicles, better incorporation of sensor data, and sharing of data through the network. With the global network in place, electronic collaboration can be carried out among distant actors, requiring an understanding of how social process such as collective decision making, team dynamics, and trust transfer from face-to-face to the digital world. Cultural factors play an integral part in social interactions, and this project will use the Culturally Infused Social Networks (CISNs) framework to realistically model individual and group behavior in Network-Centric Operations (NCO). The project will also research and develop parallel and distributed techniques to extend socio-cultural modeling for large and dynamic NCO networks. Examining social behavior under various scenarios and diverse network conditions will help the Army to refine the network infrastructure and train human operators. This project will develop modeling and simulation tools to help the Army make a smooth transition to network-centric operations.

(New project, 2010)
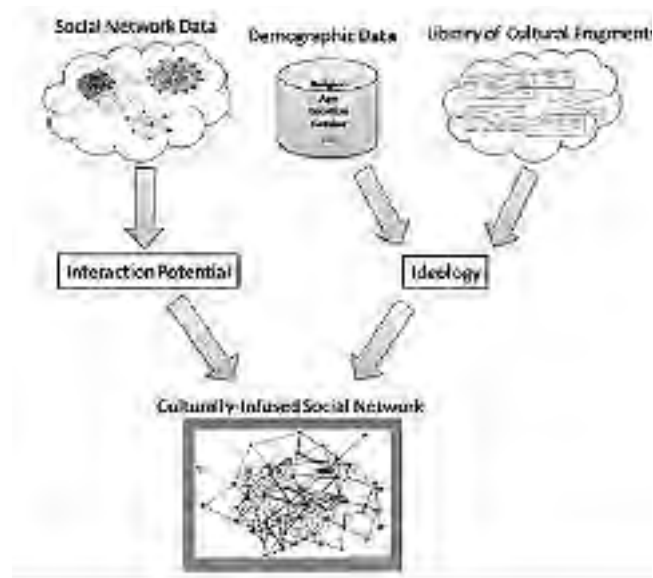
Culturally infused social network. (E. Santos, UTEP. From: Santos et al., *Proc. IC-AI Conference,* 2008)

CPI Breakdown
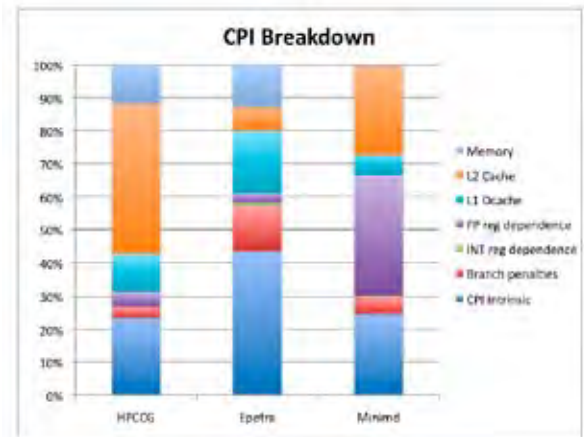
HPC Enabling Technologies and Advanced Algorithmic Development Activities

All of the AHPCRC projects rely on algorithms and computer codes that perform well on large computing clusters and supercomputers. AHPCRC computer scientists and mathematicians support these efforts and the efforts of Army researchers by developing efficient and effective algorithms, reliable and scalable computer codes and programming languages, and capabilities for analyzing machine performance.

These projects aim to create highly parallel programming environments and advanced computational algorithms to support cross-cutting areas of interest in almost all aspects of high performance computing, and the advances they provide will benefit the U.S. Army and other scientific communities. Writing efficient high performance applications requires detailed knowledge of the underlying machine's architecture. Machine architectures evolve quickly, so programs must be written to run efficiently on the next generation of hardware as well as on existing machines. AHPCRC researchers are developing the Sequoia programming language, which uses virtual memory hierarchies for portability and auto-tuning for performance optimization on specific machine architectures.

Improving performance and programmability in high performance scientific computing requires co-developing hardware systems and scientific applications that can run at full speed on large data sets. The Flexible Architecture Research Machine (FARM) is a prototyping platform for exploring new software and hardware approaches to parallel system design. FARM is being used to tackle large, complex graph analysis problems.
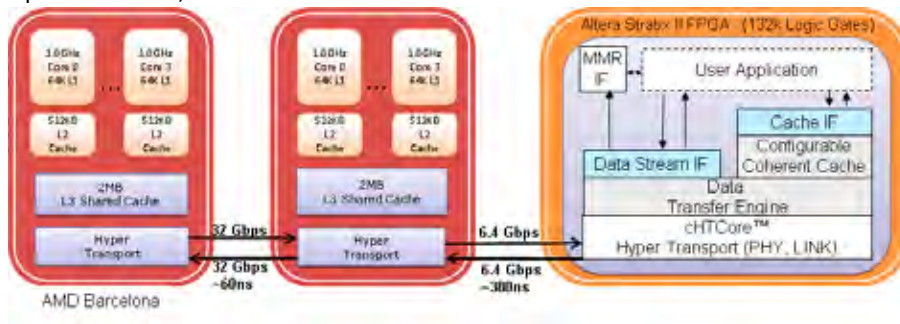
Clockwise from top left: Roadrunner Supercomputer at Los Alamos (LANL photo); System performance analysis (P. Teller, S. Arunagiri, UTEP); Flexible architecture research machine (K. Olukotun, C. Kozyrakis, Stanford); Sequoia memory hierarchy (A. Aiken, W. Dally, P. Hanrahan, Stanford); Network node graph (L. Guibas, Stanford); Permeability map (M. Argáez, L. Velázquez, UTEP); Disparity map stores depth information from stereoscopic images as gray-scale values (P. Teller, S. Arunagiri, UTEP).

Many Army applications can run more efficiently and cost-effectively on heterogeneous multicore processor systems, which are becoming more common in commercial computers.

As multicore systems become more common, and microprocessing chip power increases, so does the challenge of getting data into and out of the chip. Componentized modeling and simulation systems can be used to study the performance of large-scale heterogeneous multicore parallel computing systems to identify and remedy bottlenecks and sources of program instability.
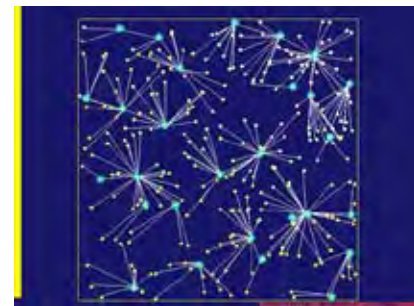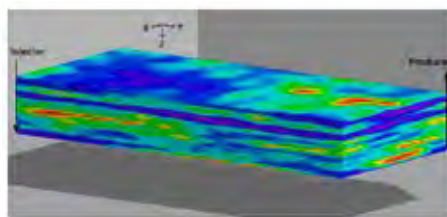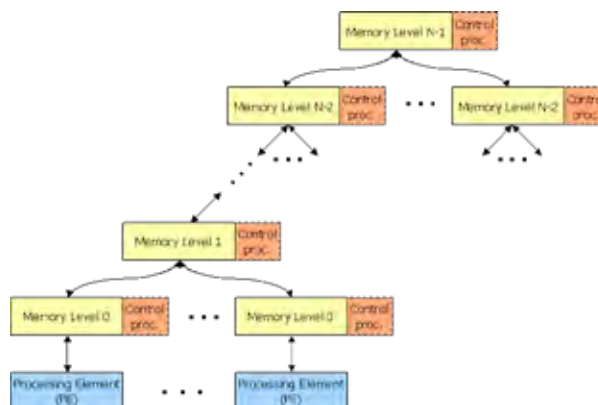
A hybrid approach to solving mathematical problems with large numbers of local minima provides flexibility and efficiency, and may lead to solutions that are not accessible by other means. Algorithms for searching parameter spaces and reducing the computational cost of solving equations can be adapted to work well in a high performance computing environment.

"The Army's scientists and engineers are expanding the limits of our understanding to provide our Soldiers, as well as our Joint and coalition partners, with technologies that enable transformational capabilities… to ensure that the Army remains a relevant, ready, and victorious land component of the Joint Force. The Army science and technology community is the 'engine' of change for the Army's transformation."
— Dr. Thomas H. Killion

Enabling HPC

Distribution Statement A: Approved for
public release; distribution is unlimited.

Project 4–1: Stream Programming for High Performance Computing

Principal Investigators: William Dally, Pat Hanrahan, and Alex Aiken
(Stanford University)

Parallel programming is an intrinsic part of high performance computing (HPC)—codes must be designed to run well on systems with tens to thousands of processors working cooperatively. Programmers must design code that fits the characteristics of a given system architecture. Code that works especially well on one architecture may not achieve the same level of performance on a system with a different size or structure. Programs written to be highly portable may not perform optimally on any system. AHPCRC researchers at Stanford University have recently released Sequoia, a programming system that facilitates writing code that is functionally correct on any system, then tuning the performance to the characteristics of a specific system. Sequoia delivers efficient performance running programs on GPUs and distributed memory clusters.

High-performance parallel architectures increase performance and efficiency by allowing software to manage a hierarchy of memories. Such systems consist of many processing elements operating in isolation, drawing data only from their own small, fast local memory devices. Data and code move between levels in the hierarchy as asynchronous block transfers explicitly orchestrated by the software. Programmers must build into the software the directives to move data between nodes at adjacent levels of the memory hierarchy. Explicit management of the memory hierarchy gives the programmer direct control over locality, allowing the programmer to improve performance by writing locality-aware programs.
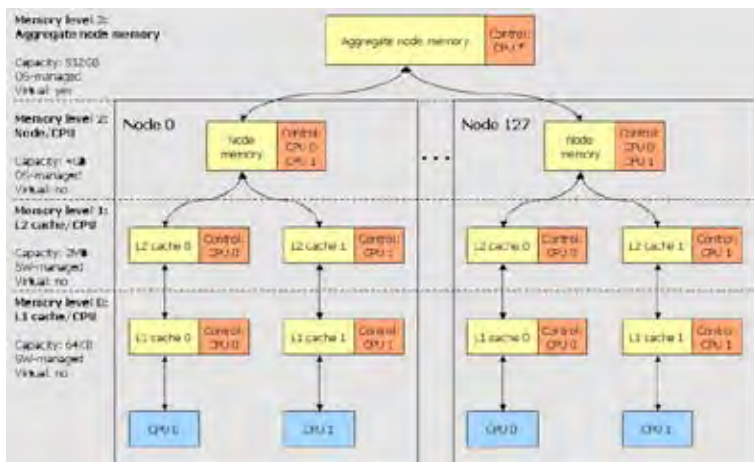
Sequoia programmers employ virtual memory hierarchies that can be mapped to specific machine architectures. (A. Aiken, Stanford University)

The Sequoia language places data movement and placement explicitly under the control of the programmer. Machine architecture is represented in the language as abstracted memory hierarchy trees. Self-contained computations called tasks are used as the basic units of computation. Tasks provide for the expression of explicit communication and locality, isolation and parallelism, algorithmic variants, and parameterization. These properties allow Sequoia programs to be portable across machines without sacrificing the ability to tune for performance. Sequoia programmers work with an abstract memory hierarchy, which does not depend on the specific memory sizes, number of computer nodes, or depth of a particular memory hierarchy. This allows a programmer a high degree of control over both the data and the parallel computation without tying a program to a particular machine architecture.

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public release; distribution is unlimited.

Enabling HPC

Project 4–2: Massive Scale Data Analysis on the Flexible Architecture Research Machine (FARM)

Principal Investigators: Kunle Olukotun and Christos Kozyrakis (Stanford University)

Graphs—a fundamental abstraction for modeling and analyzing data—are used extensively in counter-intelligence, business intelligence, data discovery, web mining, simulation data analysis, social network analysis, and bioinformatics. Graphs can represent transportation networks, communication networks, and socio-economic interactions. Graph-based models have also been used in machine learning for machine translation and robotics, and many scientific computing problems are formulated using graphs.

Because of the recent explosion in the amount of data and the complexity of the phenomena being modeled, graph representations have grown to hundreds of millions or billions of nodes. This size, combined with increasingly complex graph analysis algorithms, makes large-scale graph analysis a challenging problem. Current architectures and programming environments are not well suited to these algorithms. Large-scale graphs are not easy to partition and may require frequent updates to the graph structure
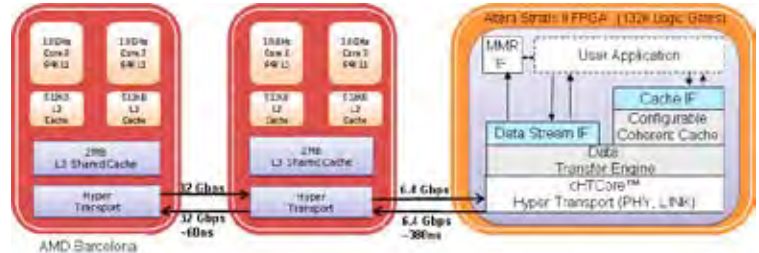
One configuration of the Flexible Architecture Research Machine. (Graphics this page: K. Olukotun, C. Kozyrakis, Stanford University)

during analysis. This makes them unsuitable for current commodity clusters, which do not provide global random memory access or enough communication bandwidth for the irregular data access required by graph algorithms.

AHPCRC researchers at Stanford are applying a platform that they developed to large-scale graph analysis problems. The Flexible Architecture Research Machine (FARM) is a flexible, high performance prototyping platform that allows researchers to demonstrate full-system prototypes running full-sized HPC applications. The FARM closely couples commodity processor and field-programmable gate array (FPGA) technologies, making it ideal for experimenting with application-specific accelerators and novel memory system designs. FARM uses a hybrid software–hardware transactional memory acceleration system that is the only hardware implementation to date that handles large transactions. The Stanford team is focusing on increasing FARM's functionality and efficiency.


Warp graph algorithms can alleviate computational work-load imbalances common to real-world skewed graphs.

Project 4–3: Specifying Computer Systems for Field-Deployable and On-Board Systems of Multicore Processors

Principal Investigators: Patricia Teller and Sarala Arunagiri (The University of Texas at El Paso)

High-performance computing (HPC) in the guise of multi-core processors, GPGPUs (general-purpose graphics processing units), FPGAs (field-programmable gate arrays), accelerators, and solid-state devices, is propelling the growth of non-traditional HPC—in particular, its use in field-deployable and on-board systems for processing sensor, signal, and image data. Such HPC-enabled systems can execute applications at extraordinary speedups, allowing some applications to migrate from larger fielded systems to smaller on-board systems, and decreasing the communication time between them. Although this can increase capability to meet operational timelines, this capability is limited by size, weight, and power (SWaP) constraints. Often, on-board systems have even stricter SWaP constraints than their fielded counterparts.

This project addresses many of the practical computational aspects of effectively employing emerging HPC technology in field-deployable and on-board systems. With system SWaP constraints in mind, AHPCRC researchers at UTEP are investigating the tradeoffs associated with executing Army-relevant applications, computational kernels, and alternative algorithms and implementations on different multi- and many-core processors. They are quantifying tradeoffs concerning execution time, parallelism, precision, memory footprint, output fidelity, power consumption, and energy efficiency, with the goal of effectively mapping applications or application segments to processor architectures. Intelligent mapping of this kind can provide valuable assistance in
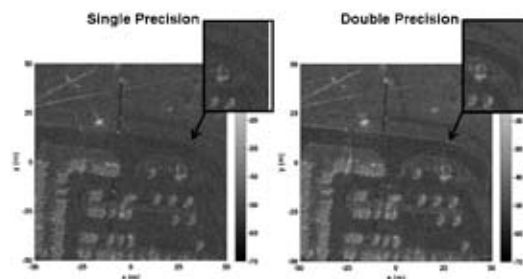
Synthetic aperture radar (SAR) images. Single-precision processing (left) may provide sufficient image resolution at a lower computational cost than double precision (right). (P. Teller, S. Arunagiri, UTEP.)

accelerating the infusion of new technologies into on-board and field-deployable HPC systems, assessing the merit of investing time in program development, and distributing workloads in heterogeneous computing environments. The longer-term goals of this work include developing models to facilitate this application-to-architecture mapping, a model to characterize application power consumption, and a methodology to adapt a program's execution intelligently and dynamically to enhance energy efficiency and, thus, extend the effective life of system operation.

Chimera, a heterogeneous computing cluster at UTEP, is being used to facilitate this research – it links various commercial multi-core processors, GPGPUs, FPGAs, and accelerators for performing vector operations. Using Chimera, the UTEP researchers, along with ARL staff, are developing tactical battlefield applications, evaluating their ability to perform well on a variety of processors, and identifying ways to reduce execution time using specialized resources.

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public release; distribution is unlimited.

Enabling HPC

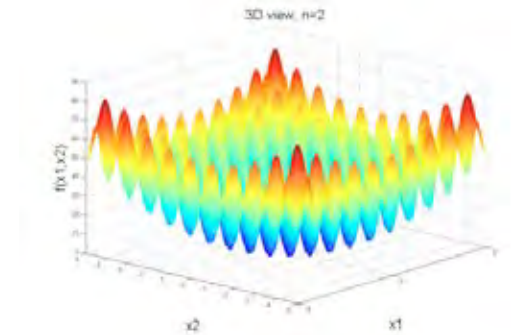# Project 4–6: Hybrid Schemes for Parameter Estimation Problems

Principal Investigators: Miguel Argáez and Leticia Velázquez
(The University of Texas at El Paso)

Effective use of the recent innovations in computer architecture can be limited by difficulties in writing functionally correct parallel applications that also achieve high performance. Hybrid algorithms combine the advantages of more than one optimization method to obtain the desired results.

The AHPCRC team at UTEP has developed a hybrid method that enables a user to choose from among several global stochastic techniques to search the parameter space for possible minima. The global search produces a set of target regions. Data points from these regions are filtered to produce a model that behaves in a mathematically similar fashion to the function of interest, while demanding less in terms of computational resources. This surrogate model is used to perform local searches, using an algorithm developed by the UTEP team. This method identifies gradients that are steep enough to lead to a lower function value. The algorithm may also include physical bounds to ensure realistic solutions.

To implement HPC applications on highly parallel systems, the UTEP team is developing a model in which transactions (individual small operations) are used to express parallelism, ensuring that interdependent operations are all either completed

A function with many local minima. (Graphics this page : M. Argáez, L. Velázquez, UTEP)

or canceled successfully. They are also developing a simple distributed-memory programming model with the capability of scaling to systems with thousands of processors.

The UTEP team is working on several applications of Army interest: flapping wing motion optimization, adaptive hydraulics modeling, epidemiological diseases, and signal processing.
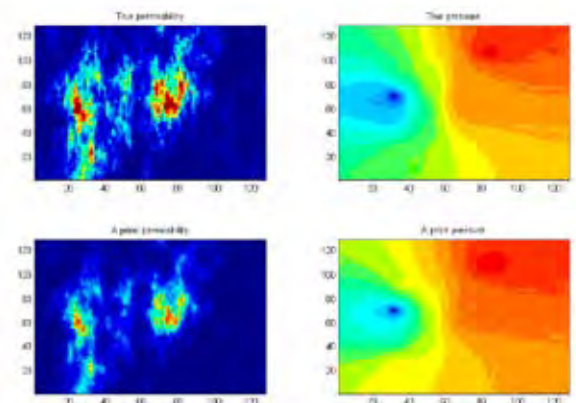

2-D hydraulic problem: permeability estimation based on pressure data. *Top:* true permeability (left), true pressure (right). *Bottom:* corresponding a priori permeability and pressure.

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University Leads,
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Project 4–1: Stream Programming for High Performance Computing
Design and compilation of parallel programming languages, static and dynamic analysis of programs, program verification.

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Project 4–6: Hybrid Optimization Schemes for Parameter Estimation Problems
Developing large-scale optimization algorithms with applications to science and engineering problems.

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Project 4–3: Specifying Computer Systems for Field-Deployable and On-Board Systems of Multicore Processors
Applications, operating systems, and computer architectures adaptations and methodologies; performance evaluation, modeling, enhancements; parallel and distributed computing; workload characterization; education.

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Project 3–4: Robust Wireless Communications in Complex Environments
Exploring how fixed and mobile ad hoc networks can be integrated and enhanced for tactical communications.

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Project 2–5: Nanoscale Dislocation Dynamics in Crystals
Predicting mechanical strength of materials through theory and simulations of defect microstructures across atomic, mesoscopic and continuum scales.

Principal Investigators

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public release; distribution is unlimited.

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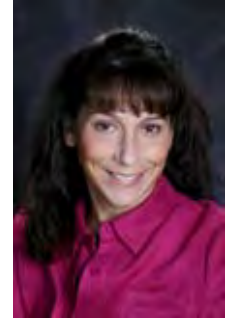
Project 4–7: Evaluating Heterogeneous High Performance Computing for Use in
Field-Deployable Systems
*Director, NMSU Advanced Computer Architecture Performance and Simulation
Laboratory. Microarchitecture and system simulation techniques, processor and system
power and performance modeling, workload characterization, power optimization
techniques.*

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Project 4–1: Stream Programming for High Performance Computing
*Streaming supercomputer development; scalability from a single chip to thousands of chips;
improving performance on a range of demanding numerical computations through combining
stream processing with a high-performance network to access a globally shared memory.*

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Projects 2–2: Micro- and Nanofluidic Simulations for BWA Sensing and Blood Additive
Development;
2–3: Design of Antimicrobial Peptides for Nanoengineered Active Coatings;
2–6: Multiscale Modeling of Materials
*Numerical techniques to reduce computational expense and enable the simulation of
large-scale systems over realistic time scales. Applications in biomolecular simulations,
electrodynamics, and acoustics.*

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Project 3–4: Robust Wireless Communications in Complex Environments
Exploring how fixed and mobile ad hoc networks can be integrated and enhanced for tactical communications.

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Projects 1–1: Multifield Simulation of Accelerated Environmental Degradation of Fabric, Composite and Metallic Shields, and Structures;
1–4: Flapping and Twisting Aeroelastic Wings for Propulsion;
1–8: High-performance computation of projectile impact with electromagnetic fabric
Mathematical models and computational methods for high-performance simulations. Multiscale methods, dynamic data-driven systems, model reduction, near-real-time computing, and large-scale engineering applications.

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Project 3–1: Information Dissemination and Aggregation under Mobility
Computer representations for sensing, modeling, manipulating, and rendering objects and processes. Structures for mobile data, image database browsing and navigation, visibility and motion planning algorithms, techniques for handling geometric data.

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Project 4–1: Stream Programming for High Performance Computing;
Rendering algorithms, high performance graphics architectures, and systems support for graphical interaction. Raster graphics systems, computer animation, and modeling and scientific visualization—volume rendering in particular.

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Project 1–5: Numerical Simulation of Flapping Flows
Aeromechanics and computational fluid dynamics.

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Project 3–3: Secure Sensor Data Dissemination and Aggregation
Wireless networks, sensor networks, and optical networks.

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Project 2–1: Dispersion of BWAs in Attack Zones
*Computational fluid dynamics of industrial problems, turbulence modeling
(RANS/LES) and numerical methods for computational fluid dynamics.*

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Project 2–1: Dispersion of BWAs in Attack Zones
*Understanding physical, chemical, and dynamical processes in the atmosphere to address
atmospheric problems such as climate change and urban air pollution, with improved
scientific insight and more accurate predictive tools.*

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Project 1–3: Multidisciplinary Parametric Modeling and L/D Quantification and
Optimization
*Numerical solution of partial differential equations with applications to subsonic,
transonic, and supersonic flow past complex configurations, as well as aerodynamic
shape optimization.*

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Project 4–2: Massive-Scale Data Analysis on the Flexible Architecture
Research Machine (FARM)
*Architectures, runtime environments, and programming models for parallel computer
systems. Transactional memory, architectural support for security, and power management
techniques.*

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Project 1–2: Simulation of Ballistic Gel Penetration
*Computational solid mechanics, material modeling, numerical analysis. Mechanics of
materials under highly dynamic deformations: impact, blasts and shocks. Interplay between
chemistry and mechanics in biology: mechanics of polymeric networks and biomaterials.*

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Project 1–5: Numerical Simulation of Flapping Flows
*Parallel code performance optimization, frameworks and runtime
systems for parallel and distributed environments.*

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Project 1–7: Advanced Optimization Algorithms and Software
*Creating, analyzing, and implementing optimization algorithms. Developing
general-purpose optimization software for the solution of practical problems.*

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Project 3–5: Mobile Brain–Machine Interface for Integrated Information–Social/
Cognitive Network Operations
*Experimental and numerical analysis of electromagnetic fields in biological bodies.
Development of forward solvers and inverse algorithms for cardiac and neural
source imaging.*

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Project 4–2: Massive-Scale Data Analysis on the Flexible Architecture
Research Machine (FARM)
*Design, performance analysis, and verification of computers. Hydra single chip
multiprocessor project and the TCC Transactional Coherence and Consistency project.
Developing novel simulation, estimation, and verification techniques for system-level design.*

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Project 2–4: Protein Structure Prediction for Virus Particles
*Logic and Constraint Programming, high performance computing, bioinformatics,
knowledge representation and reasoning, assistive technologies.*

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Project 1–6: The All-Electron Battery: Quantum Mechanics of Energy Storage
in Electron Cavities
*Scaling effects and quantum confinement phenomena for energy conversion. Mass transport
phenomena across thin membranes (oxide films and lipid bi-layers). Prototype fuel cells,
solar cells, and batteries serve to test new concepts and novel material structures.*

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Project 1–5: Numerical Simulation of Flapping Flows
*Computational fluid dynamics for application to very large scale unsteady flows
on massively parallel systems and numerical methods for computational fluid
dynamics.*
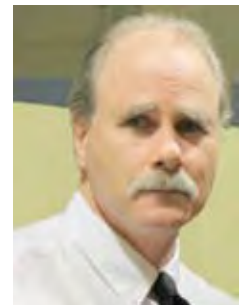
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Project 2–7: Graphene Chemistry for Electronics Applications
Ultrafast materials science and photonics, materials under extreme conditions, shock wave compression of materials, THz radiation, THz frequency acoustics, energetic materials and detonation.

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Project 3–2: Scalable Design Methods for Topology Aware Networks
Information networks, discrete mathematics and algorithms, approximation algorithms, optimization methods.

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Project 3–6: Modeling Socio-Cultural Processes in Network Centric Environments
Parallel and distributed processing, computational science, networking, socio-cultural modeling, complex adaptive systems.

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Project 1–7: Advanced Optimization Algorithms and Software
Mathematical methods for solving large-scale constrained optimization problems and large systems of equations; applications in engineering, science, and business. Co-developer of MINOS, SNOPT, SQOPT, SYMMLQ, MINRES, LSQR, and LUSOL.

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Projects 2–1: Dispersion of BWAs in Attack Zones,
2–2: Micro- and Nanofluidic Simulations for BWA Sensing and Blood Additive Development
Transport mechanics of complex fluids: large-scale simulations of poorly understood phenomena coupled with detailed experiments to elucidate the important physics in a variety of processes.

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Project 1–4: Flapping and Twisting Aeroelastic Wings for Propulsion
Theoretical and computational fluid dynamics, vortex dynamics, interactions of solid bodies with coherent vortices in fluid flows, geometric control theory with applications to spacecraft and satellite maneuvering.

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Project 1–4: Flapping and Twisting Aeroelastic Wings for Propulsion
Experimental fluid dynamics, bio-inspired flow, biofluidics, microfluidics, turbulent flow, optical metrology and development of flow diagnostic methods.

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Project 4–3: Specifying Computer Systems for Field-Deployable and On-Board Systems
Dynamic adaptation of applications, operating systems, and computer architectures; performance evaluation, modeling, and enhancements; parallel and distributed computing; computer architecture, operating systems, and simulation methodologies; workload characterization.

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Project 4–6: Hybrid Optimization Schemes for Parameter Estimation Problems
Developing high performance optimization algorithms for large-scale computational science problems.

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Project 1–4: Flapping and Twisting Aeroelastic Wings for Propulsion
Computational fluid dynamics, aeroacoustics, control and optimization, low-dimensional modeling.

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Project 3–4: Robust Wireless Communications in Complex Environments
Computational and applied electromagnetics.

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Project 1–1: Multifield Simulation of Accelerated Environmental Degradation of Fabric, Composite and Metallic Shields, and Structures
Micromechanical material design, granular flow, and the mechanics of high-strength fabric. Computational approaches for nonconvex multiscale–multiphysics inverse problems, addressing how large numbers of micro-constituents interact to produce macroscale aggregate behavior.

University Leads

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Administration and Support

BARBARA BRYAN
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Ms. Bryan, who is based at Stanford University, oversees the management of the research and outreach programs, working with the Center Director. She works with the Army and the Center Director to communicate research objectives and report on accomplishments, and to align and identify potential HPC resources on at-institution or DoD platforms. She works with each university's outreach manager and Consortium representative to establish an integrated outreach program emphasizing the Army research and HPC/computational science objectives.

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Mr. Law coordinates relations, operations, administration, and security of university-based systems for members of the AHPCRC consortium located at Stanford University. He also offers guidance and support to users of systems at the other member universities regarding compliance with AHPCRC security concerns and administration best practices. He has over 12 years experience in information technology, and has spent the past several years working in the area of high performance computing systems support.

NANCY MCGUIRE
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Dr. McGuire coordinates reports, project publications, and publicity materials for AHPCRC. She holds a Ph.D. in chemistry from Arizona State University, and she has career experience in laboratory research and scientific and technical communications. She has written and edited scientific journal manuscripts, print magazine and web content, and corporate communications materials. She has worked on website and print magazine redesign projects, and she has training and experience in website usability and content management. In addition, she has worked in media relations and represented her employers at trade shows and professional conferences.

MARK POTTS
AHPCRC Senior Computational Scientist, HPTi
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Dr. Potts has over 15 years of software development experience, including more than 12 years of work in research and application development using HPC systems. He joined HPTi in 2007 as a senior computational scientist supporting AHPCRC's academic research partners. Although the majority of Dr. Potts' research has been related to computational fluid dynamics, he also has experience in data mining, biometrics and computational finance.

Technical Areas

TA1: Lightweight Combat Systems Survivability

Strong, impact-resistant materials lighten the soldier's load, give the soldier increased protection, and minimize unnecessary risk to soldiers. Where possible, mechanical devices such as drone vehicles can stand in for humans to do hazardous or tedious work. Computer simulation allows designers to try out numerous mechanical and material configurations to see which ones work best. The resulting computational models can be applied to human tissue structures as well, enabling the development of better medical treatments and reconstructive capabilities.

TA2: Computational Nanotechnologies and Biosciences

Many important changes happen on the scale of molecules, viruses, and sub-microscopic particles. Computer simulation is ideally suited for setting up realistic scenarios and studying the interplay of many factors. High performance computing is used to design strong, lightweight materials "from the atoms up" or to model biological systems at the molecular level. The speed and capacity of massively parallel computers are key to simulating real-world phenomena on scales ranging from nanometers to city neighborhoods and nanoseconds to hours.

TA3: Computational Battlefield Network and Information Sciences

Civilian wireless communications networks must provide reliability and mobility, while accommodating many applications (voice, data, images, navigation) within available bandwidth. Military networks require all of this, plus security, stealth, resistance to hostile interference, and the ability to set up ad hoc networks in a variety of environments. Computer modeling aids in designing complex wireless communications networks for optimum security and effectiveness. HPCs incorporated into operating networks provide fine-tuning and real-time adaptability to changing circumstances.

TA4: HPC Enabling Technologies and Advanced Algorithms

As computing applications become more demanding, computers and the programs that run on them must evolve as well. This is especially true for high performance computing, where power consumption levels, computing resource usage, and program portability between platforms are essential to the effective use of these resources. Programming and algorithmic capabilities developed for AHPCRC point the way toward wider application as multicore processors and parallel programming become common in the commercial marketplace.

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Army High Performance Computing Research Center
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